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# ***JPRS Report***

# **Science & Technology**

***USSR: Chemistry***

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## SCIENCE &amp; TECHNOLOGY

## USSR: CHEMISTRY

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UDC 546.426

## DEVELOPMENT IN 1985 OF WATER ANALYSIS METHODS

Kiev KHIMIYA I TEKHNLOGIYA VODY in Russian Vol 9, No 1, Jan-Feb 87  
(manuscript received 3 Sep 86) pp 30-56

[Article by A. V. Terletskaya, Institute of Colloid Chemistry and Water Chemistry imeni A. V. Dumanskiy, UkSSR Academy of Sciences, Kiev]

[Abstract] This literature review covers works published in calendar year 1985 on the analysis of water. Determination of inorganic and organic components is discussed. Special attention is given to phenols, pesticides, surface-active agents, petroleum and petroleum products, nitrosamines, primary amines, aldehydes and other organic components. References 318: 70 Russian, 248 Western.

6508/5915  
CSO: 1841/307

UDC 543.530:669.015.4

## NEUTRON-ACTIVATION ANALYSIS OF PURE SUBSTANCES WITH USE OF HIGH-FLUX NUCLEAR REACTOR

Moscow ZHURNAL ANALITICHESKOY KHIMII in Russian Vol 42, No 2, Feb 87  
(manuscript received 22 Oct 85) pp 256-262

[Article by T. T. Kiseleva, B. S. Rabinovich, V. I. Firsov and M. N. Shchulepnikov, State Scientific-Research and Planning Institute of the Rare Metals Industry, Moscow]

[Abstract] The purpose of this work was to achieve a significant reduction in the lower limits of determination of impurities by simultaneously increasing the neutron reactor flux used in activation analysis from  $1 \cdot 10^{13}$  to  $1 \cdot 10^{14}$  neutrons  $\cdot s^{-1} \cdot cm^{-2}$ , bombardment time from 20-40 hr to 200 hr, charge of specimen analyzed to 10-20 g and activity measurement time to 6 hours. Two channels of a water-cooled, water-moderated reactor with neutron flux density  $0.4 \cdot 10^{14}$  and  $1 \cdot 10^{14}$  neutrons  $\cdot s^{-1} \cdot cm^{-2}$  were used. The increases in neutron flux, charge mass and bombardment time increased the induced activity of the



charges by 50-100 times, decreasing the lower boundary of content which can be determined by impurities in silicon, germanium and lead by 1-3 orders of magnitude, to  $10^{-9}$ - $10^{-12}$  weight percent in high purity silicon and lead,  $10^{-7}$ - $10^{-11}$  weight percent in germanium. The list of elements which can be found was also significantly increased. References 12: 9 Russian, 3 Western.

6508/5915  
CSO: 1841/306

UDC 543.544

#### USE OF HPLC FOR DETERMINATION OF GROUP V, G AND M AFLATOXINS AND THEIR METABOLITES

Moscow ZHURNAL ANALITICHESKOY KHMII in Russian Vol 42, No 2, Feb 87  
(manuscript received 23 Dec 85) pp 322-327

[Article by K. I. Eller, N. V. Rybakova and V. A. Tutelyan, Institute of Nutrition, USSR Academy of Medical Sciences, Moscow]

[Abstract] A method is suggested for normal-phase HPLC allowing simultaneous determination of  $B_1$ ,  $B_2$ ,  $G_1$ ,  $G_2$ ,  $M_1$ ,  $B_{2a}$  and  $M_{2a}$  aflatoxins with high sensitivity. The detection limit of the method is 0.1  $\mu\text{g/kg}$  for  $B_1$  and 0.02  $\mu\text{g/kg}$  for  $M_1$  aflatoxin. A mixture of ether, methanol and water 95:4:1 or 90:8:2 by volume is used as the mobile phase, and provides good quality and stability of separation parameters of the basic aflatoxins, allowing these mycotoxins to be determined with high sensitivity in the food products most frequently contaminated by them. The content of these aflatoxins and their metabolites in the animal body and tissues can also be determined by the same method. Figures 3; references 12: 1 Russian, 11 Western.

6508/5915  
CSO: 1841/306

UDC 542.61:543.38

#### EXTRACTION ISOLATION AND SEPARATE DETERMINATION OF GLYFOSATE AND DICHLOROFOS IN AQUEOUS SOLUTIONS

Moscow ZHURNAL ANALITICHESKOY KHMII in Russian Vol 42, No 2, Feb 87  
(manuscript received 13 Nov 85) pp 328-331

[Article by I. S. Shevchuk, Yu. G. Dubchenko and G. Ye. Grudneva, Donetsk State University]

[Abstract] A study is reported of the extraction of the herbicide glyfosate (GF) by organic solvents and solutions of normal primary  $C_{10}$ - $C_{14}$  alkylamine

chlorides in order to select conditions for extraction separation, concentration and determination of the herbicide in aqueous solutions. Data are also presented on the extraction of the insecticide dichlorofos to assist in selection of conditions for extraction separation of GF and dichlorofos when both are present in water. Extraction allows concentration, separation and separate determination of the two products under these conditions. Inorganic salts act on GF as salting-out agents or form complex compounds with it, increasing the degree of extraction. Extraction allows concentration and separate determination of GF and dichlorofos, decreasing the limit of detection of the pesticides to 10 and 0.3 mg/l by photometry and thin-layer chromatography. References 11: 8 Russian, 3 Western.

6508/5915

CSO: 1841/306

## 'CATALYST' INTERBRANCH SCIENTIFIC TECHNICAL COMPLEX

Moscow KHIMIYA I ZHIZN in Russian No 3, Mar 87 pp 2-11

[Article by V. Zyablov, "Catalyst"; first paragraph is introduction]

[Text] "Proceeding from the fact that accelerated development of equipment and technology requires increasing build-up of the supply of basic scientific ideas and applied developments, dramatic redirection of science to the needs of the national economy, the Plenum deems it quite important to augment the output of scientific personnel of academy, industrial and VUZ institutions in the area of tasks related to comprehensive intensification of production, improved effectiveness of the economy, to intensify integration of science with industry. More attention should be devoted to the work of scientific production associations and interbranch scientific technical complexes. Immediate steps must be taken to upgrade training of scientific personnel, augment their ranks with talented young people, provide conditions for fruitful work of scientists, increasing the equipment provisions for science and strengthening its experimental base"--decree adopted by the January (1987) Plenum of the CPSU Central Committee.

V. Zyablov, KHIMIYA I ZHIZN reporter, was told at the Institute of Catalysis at the Siberian Department of the USSR Academy of Sciences that "Development of this organization is a pressing need," in explaining the necessity of establishing the "Catalyst" Interbranch Scientific Technical Complex (MNTK). More than a literal meaning can be attributed to the name of this new association. Decisive and rapid refinement of chemical technology should become the catalyst for acceleration of scientific and technological progress outlined by the party. Let us cite only one figure: catalysts, for the production of which relatively little is spent, a few hundred million rubles per year, provide for more than 70% of the output of chemical and petrochemical products. This is an enormous figure, but in some developed countries the contribution of catalysis to the economy is even greater.

We are also faced with concrete problems that must be solved immediately.

There is a pressing need to increase the yield of clear products in petroleum refinery; here each percentage of increment is tantamount to additional extraction of 5-7 millions tons of primary raw material per year.

It is time to put order in the area of trapping and using exhaust gases in metallurgy and the chemical industry--with respect to sulfur alone, this could yield millions of additional tons annually.

Motor vehicles must be equipped with devices for afterburning exhaust gases....

It is imperative to dramatically accelerate the key link in the production chain--to develop and start using new and efficient catalysts--in order to solve this and many other economic, engineering and ecological problems.

Just how those who are working in the chief organization of MNTK, the Institute of Catalysis, are tackling this new job was discussed with this reporter by many of its staff. We submit below a report of what they told, as well as the transcript of a dialogue with Yu. Sh. Matros, doctor of engineering sciences, who is chief of the laboratory of nonstationary processes in chemical reactors.

The photos were taken by V. I. Zaykovskiy and A. L. Chuvilina, who are on the staff of the Institute of Catalysis, Siberian Department of the USSR Academy of Sciences.

#### The Tasks Are Complicated But Not Fantastic

The decision to organize the MNTK was made at the very end of 1985. Already in February 1986 there was a meeting of directors of organizations included in "Catalyst." The structure of this complex is not entirely ordinary. In addition to organizations and enterprises that are directly part of it (Institute of Catalysis, its branch in Omsk), there are also other participants. They are situated from Smolensk Oblast in the west to Irkutsk in the east, and they are subordinated to different agencies, but the MNTK program approved at the above-mentioned meeting was by no means just a good wish for them, but part of a 5-year plan which, as we know, has the force of a law. Not only chemical but instrument-making enterprises became involved in the work. For example, the Promavtomatika [Industrial Automation] NPO [scientific production association] of Groznyy undertook development and production of testing devices for industrial catalyzers.

A single chain is built: basic research--sector science--production. Of course, this is a new area, and there are plenty of difficulties and lack of coordination. There is no refined mechanism of interaction and quite a few problems have yet to be solved--not only technical ones, but financial and legal.

The first and foremost task is to put things in order, to make an inventory of what is ready in the nation, what has been produced. There are numerous organizations involved with catalysis; many developments major and minor; very much was done, and duplications were not infrequent. The scientific concept is very lofty and, in order to keep a record of it, to rule out duplication, we need an information center for catalysis, of course a modern one, based on using computers. And it is already under construction.

Another sore point is so-called introduction. There have been many miscalculations in the last few decades in the area of technical policy. It is sad to talk about this, but it has been a long time that virtually no original Soviet catalytic processes were introduced in our country. Not a single one of any major significance! We relied on importation of manufactured chemical products, and this disoriented this branch of science. It had to essentially catch up and replace foreign prototypes with domestic analogues.

We forgot how to produce testing equipment, the teams of talented people, of whom Soviet industry was proud, became scattered.... It is a truism all over the world that all major chemical enterprises must have their own "microplant" that works for the future. There was a time that we had this in our country, but the faulty set to procure ready products rendered such foresight, so to speak, superfluous.

The sophistication of enterprises producing catalysts has also become a problem. The equipment is obsolete and a significant part of it is simply inefficient. Even products that are by no means superior to the worldwide level are manufactured there at the price of utmost tension. Yet, the task was put of exceeding that level. And, in spite of all we have said, it is not considered impossible by the MNTK and USSR GKNT [State Committee for Science and Technology]. It is expected to set order in this matter within the current 5-year plan. Yet in the next 5-year plan, work will become even more complicated, we will have to indeed attain a level that exceeds the worldwide level. However, the leap that will have to be taken will not occur in empty space. Basic science was not performing so poorly, there is a concept that makes it possible to attain our goal. This applies to both the area of producing new catalysts and developing technological processes aimed at efficient use of new types of raw materials, as well as to the solution of ecological problems.

We have also seen the first concrete results achieved after organizing this MNTK. In 1986, there was intensive replacement of the catalyst generally used in the sulfuric acid industry with a new one, which was developed by the MNTK with the most active participation of the Institute of Catalysis (the very designation of the innovation--IK-1-6--[IK--Institute of Catalysis] clearly states its origin). New catalysts for polymerization of ethylene and propylene also developed here, in Novosibirsk, are also being introduced with success. Devices for catalytic purification of industrial exhaust gases have been started up at enterprises referable to the most varied ministries.

For 10 years a neutralizer, i.e., unit for afterburning of exhaust gases, could not be produced. After all, this is not such a complicated thing--a ceramic pipe with "honeycombed" interior to which a catalyst is applied. Nevertheless, for some reason it could not be manufactured sooner. In 4 months, having called upon VUZ science for assistance, suitable ceramic was produced and they learned to apply a catalyst on it by themselves. So now we have an experimental prototype of the "honeycomb." One can start producing the neutralizers, and the motor vehicle industry is probably also prepared to install them on vehicles. However, the fuel problem still remains: production of ethylated gasoline has not yet been stopped in our country, and it will not work with such vehicles; the lead it contains is toxic not only to humans, but to the catalytic device also.

There is another serious problem that it has managed to budge from a standstill: purification of exhaust gases from the Norilsk Mining and Smelting Combine. They contain many sulfur-containing elements and under the vulnerable northern conditions this presents a serious ecological problem. Work on catalytic treatment of these gases has been in progress for several years already, and by the Institute of Catalysis as well. However, the MNTK provided a powerful impetus for it: within just a few months, in

collaboration with the people in Norilsk, a pilot device was tested there, which involves a nontraditional method of reducing sulfur dioxide to elementary sulfur, the so-called liquid-phase process of Klaus. Some rather encouraging results were obtained (a commemorative medal was even cast from the sulfur thus recovered) and it has already been decided to expedite work on experimental production testing and, if it is successful, to then build a series of high-output devices.

If one wishes, important results can be achieved rapidly, even when one has to start, it would seem, at zero. But wishes alone are not enough, there must also be a material base and equipment. Two to three years ago it had everything it could dream of. Today, it is true, something more efficient has appeared in the world that Novosibirsk does not have as yet; however, very good operation of existing equipment has been attained there. A TsKP--Center for Shared Use--was organized at the institute, and more than 40 organizations of Siberia and about as many from the European part of our country call upon its services. There are times even when requests for assistance come from Moscow, where the same instruments exist, but apparently they are less accessible than those in Novosibirsk.

Kirill Ilyich Zamarayev, corresponding member of the USSR Academy of Sciences and director of the institute is to be credited with establishment of the TsKP. He assembled a team of first-rate engineers to service the unique research equipment (at the present time, this team has been made a self-contained cost-accounting department), and they have set up uninterrupted and, when necessary, around the clock operation of the instruments. The dependence of experimenters on personal connections has been eliminated: they fill contractual orders. It is planned to convert the TsKP into a VTsKP--All-Union Center for Shared [or collective] Use, and to outfit it with the latest equipment. Also, there are plans to organize an All-Union arbitration center under the MNTK to test catalysts.

Real tests require strict reproducibility, standard conditions, which are produced in automated installations that the experimental shop of the institute has. Some of them are unique in output, and they can test almost 2000 specimens per year. However, unfortunately, only a special laboratory at the institute knows how to produce such devices. The latest prototype, incidentally, is controlled by a computer which not only sets parameters, but the testing mode, adjusting itself to the properties of the catalyst. At the present time this device is being tested for a unique purpose: to detect all of the "capacities" it contains; the developers themselves still do not know all about them. An instruction model has also been produced, on which students are trained. Otherwise how could they subsequently work in modern laboratories?

True, these are small, laboratory devices. But it is a much more difficult matter with respect to larger experimental production versions.

One of the main problems is the chronic habit that ministries have of economizing on experimental production. These items are not expensive, but they create additional positions in the itemized lists of construction projects. When it is necessary to cut back expenses on new construction, this is done in

a bureaucratic fashion, by reducing first of all the number of items and, then of course, crossing out the "small stuff". One could hardly term such tactics as being farsighted.

Construction, incidentally, is a sore point also at the Institute of Catalysis. Since it became the chief organization of MNTK, of course new departments appeared for which there is no space. This means crowding. Yet no new facilities are anticipated up to the 13th Five-Year Plan. This, of course, does not facilitate acceleration of the work, but the catalysis workers have not become accustomed to complaining....

Still, they have something to be proud of. About 50 out of 71 developments deemed ready for introduction and included in the unified 5-year plan of MNTK were executed with the participation of the Institute of Catalysis, mainly in collaboration with its long-time partner (and neighbor), the SKTB of catalysts of the USSR Ministry of the Chemical Industry. Many of them are reliably ahead of what is being used in foreign industry. For this reason it can be stated with confidence that the tasks set forth are difficult but not fantastic.

#### Conservatism Is Not Synonymous With Reliability

One of the developers of nonstationary technology of catalytic processes reiterated in a conversation with reporter Yu. Sh. Matros a truth that is relevant not only to those involved in chemistry. This pioneering development is so unique that it would have been worthwhile perhaps to call it by some other name rather than merely one of the technologies. Yuriy Shayevich explained it as follows:

"We are not dealing with some individual process or even group of processes, but with an approach, a principle. Even, if you wish, with an entire philosophy....

"One can define the theoretical, ideal mode for any reaction used in industry, with which needed substances are formed with optimum yield. In real situations, an ideal is unattainable as a rule, but one can organize some optimum conditions that are close to it. How is this done? A catalyst is selected, more or less suitable working parameters--temperature, pressure, rate of delivery of basic substances and their concentration--are determined experimentally. Then they do everything they can to adhere to the set mode at any price.

"The price is often excessive. As a rule, reactions take place rather rapidly at high temperatures. What do the technologists do? They place a heat exchanger before the input to a reactor to warm the initial mixture. But the actual process usually takes place with high emission or absorption of heat, the active zone of the apparatus becomes overheated or cools, the heat has to be diverted or, on the contrary, introduced. What is done? Again, a heat exchanger is used. Then there is overheating or cooling again.... A labor-consuming, awkward and wasteful process....

"Our approach is different: the process should sustain itself. For this purpose one can, for example, provide a moving heat front in the catalyst layer, in which the required temperature is maintained in the course of the reaction

by the heat emissions during chemical conversion. And fewer heat exchangers should be used."

[Question] Is that how your "rocker," the reactor with periodic switching of flow, operates?

[Answer] "The 'rocker' is merely one version, the very first execution of the principle, but not the principle itself. It is not difficult to comprehend the arrangement of any apparatus if the substance of the process is understood. And if one begins with results, it is easy to slip into incomprehensible journalistic cliches. For this reason, I would prefer to begin with the substance.

"Movement of the heat front in the catalyst layer is a basic concept for us. It was found that the front, a narrow zone of high temperature, can be maintained even at very low baseline temperature of the mixture. It was proven that the temperature difference between the front and reactor input can be tens and even hundreds of times greater than adiabatic heating, the gradient that would be generated in an ordinary reaction. Let us consider, for example, a mixture containing only 0.1% carbon oxide. Under stationary oxidation conditions, it is capable of raising catalyst temperature by only 9 degrees. A paltry amount! But if a narrow front is produced, it may be hotter than the mixture at the input by 1000 degrees. Why?

"The fact of the matter is that heat is emitted in a narrow zone in a heat front, and is virtually not diverted from there, since this front moves at about the same speed as heat diversion. It is very low, since there are substantial differences in heat capacity of the catalyst and gas. It is higher by a factor of  $10^3$  for solids. For this reason, the mixture blown through it rapidly so to speak pumps heat in the slowly moving heat front".

[Question] But the front does advance....

[Answer] "Of course, and someday it will 'crawl' to the end. There, so as not to lose the front, time itself changes the direction of flow and directs the mixture toward it, then the front will move in the opposite direction at the same leisurely pace. This is how the function of our 'rockers' is organized: there are switches that periodically alter the direction of the gas mixture. But there can be other variants, for example, a 'doughnut' filled with catalyst, in which the front ambles in a circle without changing direction".

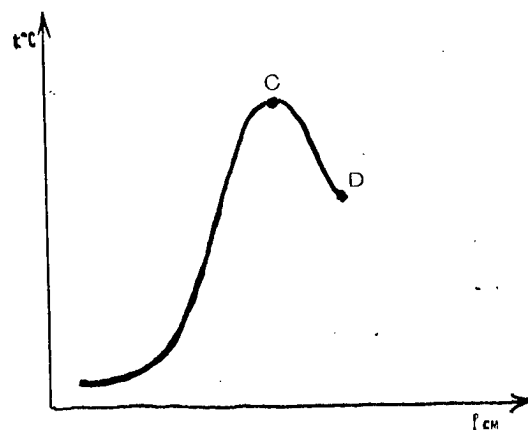
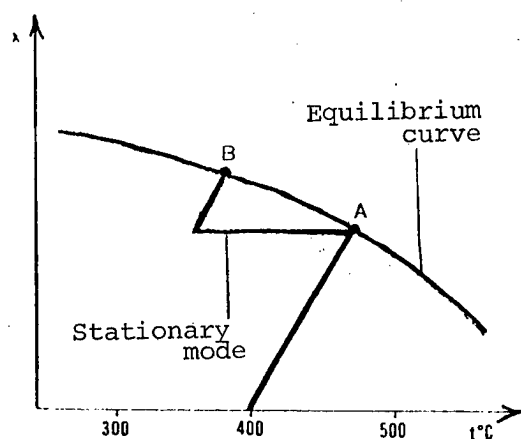
[Question] Is there not a similarity here with homeostasis that is maintained in a living system? Old-fashioned technology functions like a mediocre physician--it uses only a thermometer and fights only for a normal temperature. Yet the body is multifunctional and it can be controlled by exerting an influence on the most varied parameters....

[Answer] "Perhaps, homeostasis can also serve as a work of art. But I would put it more simply. Stationary conditions are dogmatic; they cause rigidity of all functional links. Naturally occurring systems, however, have diverse flexible mechanisms of regulation; in this respect, traditional technological



systems were inferior to them, and for this reason were incapable of achieving modes that would be close enough to ideal.

"Let me plot a textbook curve: change in equilibrated state of mixture as a function of temperature. The extent of conversion in the course of any reversible reaction (and most catalytic processes are reversible) is limited by this curve under any conditions. No matter what the baseline composition of a mixture, initial temperature this 'x' or extent of conversion changes so long as the rate of the direct reaction does not equal the rate of the reverse reaction. And that's all! You take a mixture heated, for example, to 400°C, and reached this fateful curve at point A. Then the situation is hopeless: one can increase conversion only by diverting heat. This is why stationary technology generated heat exchangers....



Extent of conversion ( $x$ ) as a function of temperature. Traditional stationary mode permitted approximation to the optimum, equilibrium curve only at certain points (A and B). Change in temperature is regulated by heat exchangers and is described by the interrupted zigzag line

Change in temperature along layer of catalyst ( $l$ --length) in non-stationary mode. The moving heat front is characterized by a maximum, point C, after which the temperature drops

"In the nonstationary mode, when there is a narrow heat front, the temperature along the catalyst layer changes uniquely; there is a section on the curve, CD, where it drops. But since this curve is such, another showing how conversion changes will rise in this segment.

"However, on the extent of conversion-temperature curve, the nonstationary mode is described by an arc-shaped curve, the top branch of which (did you notice?) is very close to the ideal, equilibrated curve (see next page--ed.).

"In addition, consider the fact that there are dynamic processes on the surface of the catalyst also, it is transformed reorganized in the course of the process. Traditional theory silently assumed that nothing happens to it, but this is far from the truth. At our institute such changes are undergoing vigorous investigation, and the prospects of controlling surface dynamics are very real".

[Question] How did you arrive at such important decisions?

[Answer] "It was a lengthy process. In the 1960's, we began with a special, purely research problem, we analyzed the operation of industrial reactors that functioned under undesirable, nonstationary conditions for different reasons; the load, composition, concentration and activity of catalyst were changed. In addition, dynamic modes turned out to be more convenient for experiments, since they made it possible to gain deeper and clearer knowledge about the physicochemical patterns of processes occurring in the reactor. Results were obtained more quickly. We began to develop mathematical models of the reactor. Then, already in the 1970's, we discovered that the dynamic mode enables us to come closer to the optimum in some situations than the stationary mode.

"We reported to the scientific council of our institute in 1975.... At first, there was only one person who upheld our conclusions, the late director of the institute, Academician Boreskov".

[Question] He was also your supervisor?

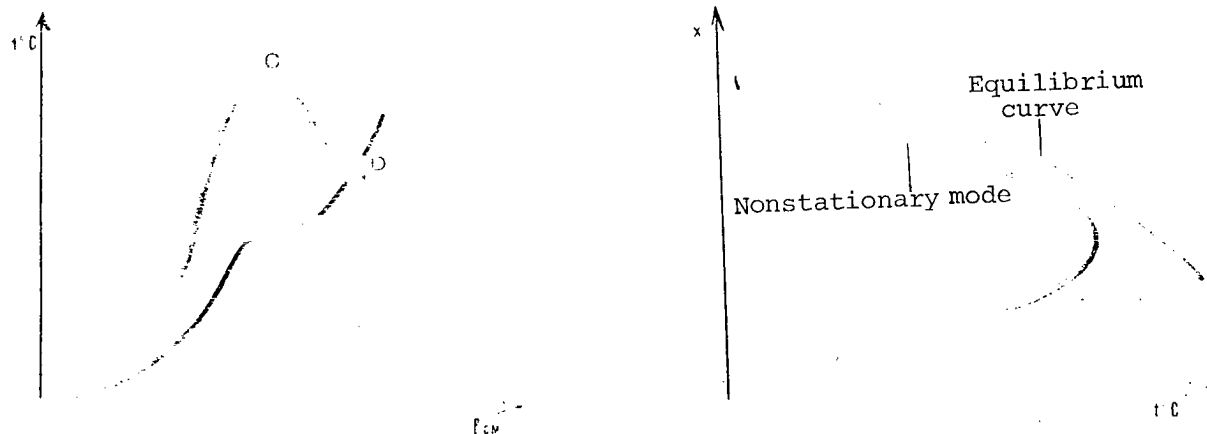
[Answer] "I would not like to refer to Georgiy Konstantinovich using this stereotype word. When speaking about research, this is how one often refers to a chief who merely signs papers without delving into things. Boreskov, however, offered genuinely creative participation in the work, he was not a supervisor, he was a friend, a colleague. For this reason he stood up for us not only passionately, but competently. We were able to continue with our work, and 7 years later our apparatus started to function at the plant. The nonstationary mode turned out to be particularly efficient when there were small amounts of initial substances, when the composition of mixtures varied. And such mixtures are extremely widespread. This applies to both industrial gas exhaust that poisons our habitat and the exhaust sulfur-containing gases of the nonferrous metallurgical enterprises. Just what we did not know how to control".

[Question] There has been an article in our journal about your apparatus, which was installed at the Alaverdy Mining and Smelting Combine, the title was "One Can Reach an Agreement With Procrustes."

[Answer] "Perhaps, conservative technology is indeed akin to Procrustes. However, it is significant too that we succeeded in reaching an agreement, to find a language in common with the production people, the specialists at the Krasnoural Copper Smelting Combine, who became our co-authors in the first introduction of this innovation. I shall not dwell on the details (there were also some clashes), but as a result of this collaboration, a device was started up in 1982 that processes 40,000 m<sup>3</sup>/h converted gases with SO<sub>2</sub> content ranging from 1 to 4%. This gas, which previously generated acid rain, began to be processed into marketable sulfuric acid.

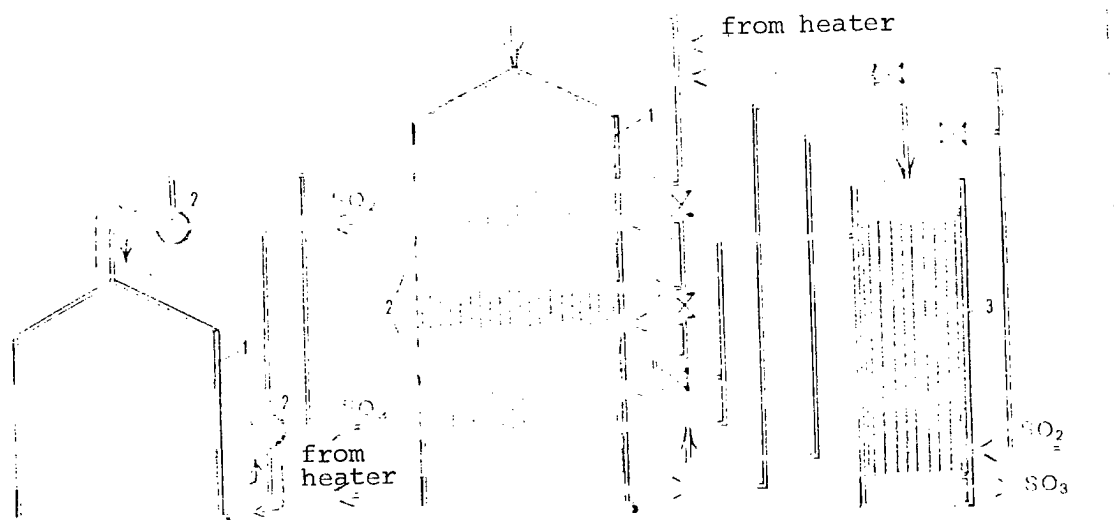
"The most superficial comparison of the methods will convince you that the system with 'rocker' is much more efficient than the traditional method. You will see immediately that the nonstationary processes requires much less equipment. A comparison of quantitative indicators yields an even more convincing result. Several times less metal is used with the 'rocker' than with the old model of contact apparatus; for this reason it offers half the hydraulic

resistance to the flow of gas (and to overcome resistance means that energy has to be expended for gas blowers); capital and operating expenses with the 'rocker' are one-third to one-fourth the former level, and there is zero fuel expenditure for heating.



Curve with inflection superposed on plot illustrated in preceding figure--change in extent of conversion ( $x$ ) along catalyst layer in nonstationary mode. In segment CD,  $x$  starts to grow again

Extent of conversion as a function of temperature changes in nonstationary mode following a curve the top branch of which is close to optimal



Reactors with equal output illustrated on the same scale. On the left--functioning in nonstationary mode, on the right--traditional, stationary mode. Contact unit of the second one consists of reactor 1 (4 layers of catalyst), intermediate heat exchangers 2 and preheat exchanger 3. The contact unit in nonstationary mode consists of reactor 1 with a single catalyst layer and (key element in the system) high-speed 3-way valves 2, which switch direction of gas flow

"At the present time there are such units in operation at four metallurgical plants, and very soon they will be installed at four more. There is no longer any justification for complaining about the conservatism of production workers, there are more proposals to collaborate than we can handle. We, it can be said, are slowing things down ourselves, because we simply do not have time to respond to all requests".

[Question] You have been talking about oxidation of  $\text{SO}_2$ , about the sulfuric acid industry. But what other processes can be converted to the nonstationary mode?

[Answer] "With respect to sulfuric acid, virtually everything is clear. We are preparing for future and rapid introduction of the method to practical use, together with organizations of the Ministry for Production of Mineral Fertilizers, Ministry of Nonferrous Metallurgy, Ministry of the Chemical Industry (especially with the Mineral Fertilizer Scientific Production Association, State Institute of Nonferrous Metallurgy, SKTB of Catalysts). At present, we are pursuing, together with branch institutes, development of such processes as synthesis of ammonia, methanol...."

[Question] Is there something like this abroad?

[Answer] "The priority of our country is protected by USSR author certificates, United States, English, French and Japanese patents.... Of course, publications about our developments have drawn the attention of foreign firms; however, I wish to note that the nonstationary mode is not a thing that can be "grasped" by the trial and error method that is customary to technologists. This is essentially unlikely; theoretical developments, packages of computer programs are needed. Things that only we have for the time being".

[Question] You are not worried about our priority?

[Answer] "No, not for the next few years. But to bring technological modes close to optimum means to gain billions, and not millions, on the scale of the national economy. One does not have to be an outstanding specialist to understand this. For this reason, if the new developments will start to be used in our country at the pace that has prevailed until recently, there is a possibility of again joining the ranks of those who have to catch up. However, there are grounds to expect that this will not happen this time".

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## RESTRUCTURING OF COMMERCIAL CATALYST PRODUCTION

Moscow KHIMICHESKAYA PROMYSHLENNOST in Russian No 3, Mar 87, pp 140-143

[Article by G. T. Gazaryan and A. A. Zalevskiy]

[Abstract] Catalyst production in the USSR cannot be regarded as an industry per se, but as a component of other processing and manufacturing establishments. As a result, administrative difficulties are encountered that render streamlining and overall planning difficult. In addition, many of the plants are low-volume operations that are heavy on manual labor and, as a result, operate in a low-efficiency mode. Resolution of these problems requires that proper administrative measures be taken to reassess the status of industrial-scale catalyst production, with a view toward consolidation of small operations, introduction of automation to optimize labor productivity and cost effectiveness, and increasing the quality of the products to make them more competitive abroad. References: 8 Russian.

12172/5915

CSO: 1841/293

UDC 541.128.3:541.183:539.89:[542.943.7:546.262.3]

## MECHANOCHEMISTRY. CATALYSIS. CATALYSTS

Moscow KINETIKA I KATALIZ in Russian Vol 28, No 1, Jan-Feb 87  
(manuscript received 23 Jun 86) pp 5-19

[Article by P. Yu. Butyagin, Institute of Chemical Physics, USSR Academy of Sciences, Moscow]

[Abstract] This article, a portion of the materials of the sixth All-Union Conference on the Mechanism of Catalytic Reactions, held in Moscow, 1986, discusses the physical principles of mechanochemistry and the causes of initiation and acceleration of chemical reactions during mechanical processing of solids. The phenomenon of mechanical catalysis is described, the nature of active centers investigated and mechanically-activated chemisorption of gases on fracture and friction surfaces of solids is studied. The possibility of

using the methods of mechanochemistry in processes of catalyst preparation is analyzed for the reactions of decomposition of inorganic compounds and solid-phase synthesis. Figures 9; references 58: 51 Russian, 7 Western.

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CHEMICAL-INDUSTRY MINISTER ON OVERCOMING SECTOR'S SHORTFALL

Moscow EKONOMICHESKAYA GAZETA in Russian No 16, Apr 87

[Comments by Yu.A. Besspalov, USSR minister of chemical industry, on overcoming chemical industry's lag: "The Chemical Industry"; first paragraph is source introduction]

[Text] USSR Minister of the Chemical Industry Yu. A. Besspalov describes how the sector's enterprises are overcoming their lag:

"I shall speak frankly: at the start of the year, the sector found itself in a difficult situation. In January, it had reached a production-output shortfall of 76 billion rubles. I don't want to plead weather conditions as some managers on occasion are guilty of doing in covering up their own inefficiency, but one cannot deal in silence with those severe winter trials of transport and breakdowns in the supply of power and raw materials. Under these conditions, our enterprises, due to the specific nature of their technology, particularly acutely experienced operational irregularity. Thus, because of a mishap at the local TETs, plants at the Kazan Orgsintez Association thawed. As a result, we lost 12,000 tons of polyethylene. But prompt and well-coordinated actions by the collective made it possible to prevent equipment from going out of operation and in the shortest possible time to get normal production operation reestablished. This is not the only example.

"The entire group of our subcontractors operated punctually. They are the Ministry of Petroleum Refining and Petrochemical Industry, the Ministry of Production of Mineral Fertilizers and the Ministry of Timber, Pulp and Paper and Wood Processing Industry. Joint-work schedules were compiled which are being fulfilled even now, and all activities are precisely coordinated.

"This is an important factor contributing to making up lost time. It is also important that the work experience during a difficult time does not go unnoticed. We have learned with our contractors to quickly overcome in a number of cases those vaunted interdepartmental barriers and to fight against formalism and paper shuffling in our relations.

"But let's go back to January, our most difficult month in recent years. The sector was brutally criticized, and it must be acknowledged that the

criticism was justified. The fact is that in addition to a lag in volume we fulfilled at that time the targets for only 8 out of 44 basic positions of the product list. If we were to take into account that the Ministry of Chemical Industry puts out 52,000 product designations, the indebtedness was great both with respect to a number of sectors and with respect to individual customers who also were very concerned about shortage of raw materials. In such a situation, we selected priority directions of work and effectively reorganized a number of enterprises to put out those products which customers like machine builders needed first of all. Today we are striving with all our energies to rectify the situation in other directions as well--the schedule now includes two-thirds of the product designations.

"Unfortunately, in this difficult situation we also were left without an important raw material--vegetable oil. Yet the cause here does not lie in snowdrifts but in lack of coordination of the plan for material and technical support. For an entire month--from 15 December to the middle of January--no oil was delivered. The supply planning organization was trying to decide all this time whether or not to give it to us, and if they were to give it, then how much. Yet this oil is essential for the production of paint and varnish materials.

"As a result, a large indebtedness was created in regard to this product, which is needed by many sectors. It is true that we have now reduced the shortfall from 60,000 to 39,000 tons and we continue to make up what was omitted, but this could have been entirely avoided. In order to increase production of the materials, a number of collectives made use of their internal reserves. Thus, at the Cherkessk Paint and Varnish Plant, they learned how to extract raw materials from waste. Today their experience is being adopted by other enterprises. But the problem of supply is not being solved in its entirety. Will USSR Gosplan and USSR Gosstrib take this lesson into consideration for the future? The fact is that the sector with their 'help' began 1987 with a plan that was not balanced with respect to material resources in the amount of 2 billion rubles. And to this moment the fate of 700 million of this amount has not been decided on.

"But one thing is very important--not to forget the experience of setbacks. In preparing for the winter--and we knew that it was going to be a difficult one--defects were analyzed in the work which occurred during the heavy frosts of 1979-1980 when many enterprises stopped operating for a long time. This time it did not occur: the stoppages did not exceed several days.

"It is natural that the reorganization of their work and the transition to the new conditions of management have had their effect. Enterprises came out of a difficult situation with minimal losses and are now confidently making up for the lag. Even last year, prerequisites were created for moving ahead: all production growth came from growth of labor productivity. Moreover, this was achieved with reduction of the number of persons working.

"Still another economic indicator is important--the attained correlation between the growth rate of labor productivity and growth of wages was 0.45 instead of 0.6 according to the plan. Behind these dry statistical figures is the strenuous labor of tens of thousands of people who are working under the



new conditions of management with great independence, and this means with a big return for the state and for themselves.

"Under present conditions, enterprises have the right to utilize savings from the wage fund as they wish. At the Karbolit Association in the Moscow area, the new wage conditions have already been introduced. Higher wage rates have been instituted, which is perfectly justified by the economic position of the leading enterprise.

"There are many such collectives. Through their efforts, the sector attained plan and then above-plan positions. Figures on the rate of production growth eloquently speak of the work dynamics of chemical workers: as opposed to a planned growth of 6.7 percent, an 8.6-percent growth was attained in March.

"Without a doubt, all this puts our people into a happy mood but provides no excuse for complacency: it is imperative to overcome the lag. Economic analysis of prospects and a high level of the labor excitement of socialist competition in the collectives provide a basis for the conclusion: we shall shortly make up the gap. And the generated tempo will make it possible to take the lead".

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CSO: 1841/291

FINE ORGANIC SYNTHESIS: BASIS OF EVERYTHING

Moscow KHIMIYA I ZHIZN in Russian No 3, Mar 87 pp 15-20

[Article by A. F. Pozharskiy, doctor of chemical sciences, Rostov State University, "Fine Organic Synthesis is the Basis of Everything--Topic of the Day"]

[Text] The desire to write this article came to me in 1985, following the Third All-Union Conference on Problems of Higher University Education in Chemistry. On the whole, this well-organized conference, which convened in Kishinev, was quite beneficial. But we were amazed by the fact that not a single official representative of the USSR Ministry of VUZ [higher educational institutions] was in attendance, so that all of the appeals and suggestions that emerged from time to time were left dangling, and speakers, with few exceptions, virtually failed to touch upon chemistry as such, if we construe it, as before, as the discipline dealing with substances and their conversions.

There was mainly talk about introduction into the educational process of computers and quantum mechanical calculations, instruction dealing with problems, the link with secondary school, environmental protection. All these issues are certainly important, they are in the spirit of our times, but still, somehow I felt awkward. I was thinking, is it not in the flasks of chemists concerned with synthesis that new pesticides and drugs, high-strength construction materials and chemical fibers, vivid dyes and components of electronic equipment are generated today, as they were yesterday?

The Main Task for Chemistry

As I returned from the conference, I decided to question my chemist friends: What do they see as the main objective of their discipline? This was by no means a rhetorical question. On the one hand, an answer is important from the professional point of view, in order to comprehend the hierarchy of values in our science. On the other hand, an answer is mandatory for the state agencies upon which the planning and financing of chemical research depend.

The first answer was that monitoring of production processes is the main thing for chemistry. In other responses, there were essentially variations of different practical needs: providing the public with foodstuffs, energy, etc. It would be hard to make any objection to such noble tasks and, of course they must stand at the cutting edge of chemistry. But these problems

are also being solved by many other disciplines. This means that such responses do not reflect the internal substance of chemistry, its development as a basic discipline.

The main task for chemistry, around which all the rest should revolve, can be formulated rather simply: It consisted, consists and will consist in the foreseeable future of developing new substances with beneficial practical qualities.

If we were to glance at the causes of the periodic leaps in development of civilization on earth, it is not difficult to discern two main lines. One of them is related to achievements in acquiring new sources of energy; the other, to development of new materials that furnish people with new work tools and new consumer goods. In this sense, the 20th century can be justifiably called not only the century of atomic energy, but the century of universal use of chemistry in the economy and everyday life. Indeed, even now, the share of purely chemical goods in the gross national product of industrially developed countries constitutes 10-15%; it is also planned to raise this indicator by another 8% by the year 2000, in accordance with the recently approved "Integrated Program for Use of Chemistry in the USSR National Economy."

Virtually every new chemical technological process is born in the flask of the synthetic chemist, on his laboratory table. He is concerned with development of new chemical compounds, elaboration or refinement of methods for synthesis of already known substances. This type of work is called fine organic synthesis.

Here, the word, fine, has a dual meaning. In the first place, it draws a purely formal line between laboratory experiments, where the chemists work with grams and even milligrams of substances, and a large scale industrial process, where amounts are counted in thousands of tons. In the second place, the definition of the word, fine, reflects the fact that such synthesis is in some way similar to an art: it requires intuition, imagination and exceptionally exquisite labor-consuming work. In just the same way, in the chemical industry, the term fine organic (or inorganic) synthesis refers to complicated, multi-stage processes in which kilograms or even grams of substances are involved, rather than tons.

Thus, while we recognize chemistry as one of the bases of the present civilization, within chemistry itself we must recognize the leading role of fine, primarily organic synthesis.

#### Surrender of Positions

There is no doubt that the closest link exists between the overall sophistication of the chemical industry and level of development of fine organic synthesis. The experience gained by all industrially developed countries convinces us of this. If, however, such a correspondence does not exist, the situation with organic synthesis must be considered poor. It is expressly such a poor situation that became formed at present in our country.

Let us be frank: although Soviet chemists do hold leading positions in some branches of organic chemistry (for example, chemistry of steroids, carbohydrates),

the vast majority of the greatest synthetic discoveries of the last 20-25 years were made without their noticeable participation. Let us recall for example the recovery of compounds with fluctuating bonds, valence isomers of benzene and other aromatic compounds, annulenes, configured hydrocarbons (how invaluable, for example, the synthesis of dodecahedrane, a hydrocarbon with the structure of a dodecahedron), crown-esters, numerous naturally occurring compounds (chlorophyll, vitamin B<sub>12</sub>, insect pheromones, complex antibiotics, etc.). Some of these synthetics did not have any obvious practical significance, but they were the basis for development of the most exquisite synthetic methods; in the course of this research some highly selective reagents were discovered, the strategy was formed for solving complicated problems. It is obvious that the specialists in synthetics who reached such heights are up to solving other extremely difficult problems, including practical ones.

Just when and how did we digress from the traditions of the once universally illustrious synthetic school? This sad process of surrendering conquered positions apparently began in the early 1960's. At that time, many of our laboratories started to become equipped with instruments: first ultraviolet and infrared spectrometers, then came the turn of nuclear magnetic resonance, electron spin resonance and mass spectrometers. Computers gained increasing use, there was rapid growth in popularity of quantum mechanics calculations. In principle, this was a progressive phenomenon, since there was rapid development of quantitative investigations, theory of organic chemistry as a whole, and physical organic chemistry emerged as an independent entity. This author experienced the definitely beneficial influence of these changes, which transformed the very mind set of organic chemists.

But these changes turned out to be also fraught with treacherous traps. It became possible to rapidly and safely obtain scientific results with the help of instruments and computers, not only without synthesizing compounds, but sometimes even doing without them. A conception was generated, according to which the era of synthetic chemistry is supposedly on the wane, that in the not very distant time it will be possible to "compute" any reaction with a computer and that, in general, too many substances have already been synthesized, and it is now time to submit them to comprehensive investigation, time for quantitative studies. For synthetic chemists, such talk led to an acute deficiency syndrome: even with availability of high-quality synthetic data, they began to strive toward "embellishing" their work with quantum mechanics calculations and physicochemical excesses regardless of whether this was necessary or not.

The increase in number of computer and physicochemical studies to the detriment of synthesis began to be associated with disproportionately rapid growth in number of specialists in the relevant field, and this was even reflected in academy institutions. As a result, entire staffs began to switch from organic synthesis to a more "profitable" form of work. Some time ago, for example, a docent in the department of organic chemistry at one of our respected universities told this author that their department has changed over entirely to so-called correlation analysis, since it had become difficult to achieve something of value in organic synthesis, especially by the small work force of VUZ's.

Thus, dry branches began to appear, one after the other, on the tree of our organic synthesis. The consequences were not slow in affecting allied disciplines, since the need for sensitive analytical reagents of analytic chemists, for original ligands by physical chemists, anti-corrosion and other ancillary substances for electrochemists, agents for biological research by biologists, etc., etc., ceased to be met. Agriculture, industry and electronic engineering began to experience an acute shortage of chemicals. As a result, our country must now pay for oversights in management of basic research in millions of "nonexchange" rubles to import the missing chemical goods.

In August 1986, there was a very successful Sixth International Conference on Organic Synthesis in Moscow. It demonstrated the enormous achievements and possibilities of organic synthesis. However, we shall not dwell on its scientific results. We view the main benefit of the conference in that it vividly shed light on the weak points in our science.

At the present time, the greatest worldwide achievements in organic synthesis are related to multi-stage recovery of either the most complex naturally occurring compounds, or compounds with unique structure. To perform this work, large groups of workers are being formed, usually numbering several dozen people (for example, at one time, more than 100 synthetic chemists were working on synthesis of vitamin B<sub>12</sub>), which makes it possible to reach set goals in rather short periods of time. The problem with our organic synthesis is that, while there are good schools of synthesis and talented scientists, our chemists work in small groups and their goals are, at best, to solve problems of average difficulty, and they virtually fail to reach toward the solution of genuinely pioneering problems. This is related chiefly to the poor material base of research, flaws in personnel training and unsatisfactory organization of labor.

#### Reagents

It must be said that the fad for instrumentation and computer chemistry (this author prefers to call it dry chemistry) has made an impact on the entire nation. But why did the above-mentioned negative tendencies appear expressly in our country with particular acuity?

First of all, the fact that chemists stopped working on synthesis resulted in extremely poor supply of Soviet science with respect to reagents, which are truly the "staple" of synthetic chemistry. It is one thing when it is sufficient to stretch out one's arm and take a substance, as they say, from the shelf in order to undertake the implementation of an interesting idea, and a very different matter when one must spend many weeks on uninteresting and unproductive work to obtain the initial substance. At least 15 different chemicals are needed for synthesis involving only 5-6 stages, i.e., synthesis that is primitive according to present standards; yet, considering the always needed testing of different variants, we can easily double this number. Can you imagine the time preparatory work would require if we had to prepare all these materials by ourselves?

The specifics of industrial production of reagents lie in the fact that, while the product list is very long, each substance must be produced in relatively small amounts. There may be tons, but there may also be kilograms and

even grams. M. S. Gorbachev commented on the increasing role of this branch of chemistry in the national economy at a conference of the CPSU Central Committee dealing with acceleration of scientific and technological progress (June 1985): "There is a genuine boom building up in the area of small-scale chemistry, production of pure and ultrapure materials, which largely determine the sophistication of modern engineering. For this reason, efforts must be doubled, tripled, so as not to be left behind." And what is the situation now in our country with respect to reagents?

First of all, without touching upon issues of quality (this would be the topic of a special discussion), let us indicate that there is a poor assortment of chemical reagents offered by bases and shops of Soyuzreaktiv [All-Union Reagent Trust]. They usually do not include chemicals that are difficult to produce, but nevertheless are sorely needed in the laboratory. It should also be noted that the sale of reagents is very poorly organized. Foreign firms send out, very willingly (and often free of cost), thick and colorful catalogues of the reagents they produce, and they constantly advertise their products (particularly new ones) in scientific periodicals. The reagents themselves, are shipped out within a few days after receipt of an order, in extreme cases within a month. Unfortunately, nothing like this exists in the operation of Soyuzreaktiv. The rank and file chemist is virtually deprived of information about new reagents being produced in view of the absence of advertising and unavailability of catalogues. As a result, although many reagents are manufactured in our country, one can procure them in significant quantities only if one has connections.

The most intolerable situation has developed with respect to delivery of orders. In the course of experimental research, new ideas that require immediate use of unforeseen reagents always come up suddenly. This occurs as a result of a chance observation, discussion or scientific publication of a work by a colleague. Yet Soyuzreaktiv demands that everything be anticipated and that orders be submitted ... a year in advance. But even in this case, as shown by practice, there is absolutely no guarantee that an order will be filled.

It is obvious that with such a state of affairs one can hardly tackle really large-scale synthetic tasks and succeed in competing with foreign scientists. Could this be the reason that, in recent years, there has been such an increase in share of work on synthesis that copies discoveries made elsewhere or that amounts to synthesis of new substances, but of an existing type and readily accessible, using known methods? Such unsubstantiality has even led, to some extent, to devaluation of the very concept of fine organic synthesis.

In concluding the discussion of reagents, we should also mention the fact that the All-Union program, "Reagents," was formed several years ago to improve their production. According to this program, the teams of synthetic chemists scattered over different VUZ's took on production of ordered reagents on a contractual basis. Although the Reagents program did improve the situation somewhat, there can be no talk of radical changes. As before, there is no good advertising; chemists involved in the program often do not have the necessary qualifications and themselves experience a shortage of basic reagents and necessary equipment. The variety of produced reagents is determined more by the producers than the consumers, and the former, of course,

strive to produce what is simpler for them. From the standpoint of this author, the problem can be solved only by establishing several cost-accounting and competing scientific production associations in the nation, on the basis of existing but reorganized chemical reagent plants.

### Equipment

Along with the reagent problem, there is another, equally important one--the problem of backing up synthetic research with modern equipment. Unfortunately, there is a vast rift between supplying laboratories in academy and certain departmental institutes, on the one hand, and VUZ's on the other. This causes considerable detriment to Soviet science as a whole, since many qualified specialists work at VUZ's and cadres of synthetic chemists are trained there.

Of course, modern instruments are often very expensive, and it is hardly feasible to furnish all laboratories with them. But it is absolutely necessary for each VUZ department where conditions are right for the flourishing of organic synthesis (personnel, traditions) to be equipped with at least the minimum quantity of instruments; for example, ultraviolet and infrared spectrometers, gas and liquid chromatographs, equipment for fine-layer chromatography, tables for measuring melting point, good vacuum pumps, precise microbalances, etc. Even the supply of chemical glassware cannot be considered satisfactory; we should like to stress in particular the need to furnish VUZ laboratories with sets of slide microglassware. It is virtually lacking at VUZ's although use of microglassware allows for a great savings in reagents, improves sophistication and productivity of labor.

As for expensive instruments that are difficult to operate, such as nuclear magnetic resonance spectrometers, mass spectrometers, devices for x-ray diffraction analysis, it is time to develop a branched service, which would make the necessary measurements, on a cost-accounting basis, for all who need them. We have been talking about this for a long time, but there has been no progress.

### Personnel

With reference to the "Combined Program for Use of Chemicals in the National Economy of the USSR," we should clearly realize that its success depends not only on capital investments for construction of new enterprises and updating old ones, but, to an enormous extent, on the training of qualified personnel, chiefly technological engineers and synthetic chemists. Otherwise, where would the substances come, without which there is neither chemistry nor all it can offer the national economy?

Let us recall that organic synthesis is not only a science, but a fine art, for which one must have talent and conditions for its development. A skillful creatively working synthetic chemist develops in more than 1 year of intensive and systematic work in a laboratory.

In most cases, good synthetic chemists are trained at the nation's universities and, in part, at chemical-technological and polytechnical institutes. The first task is to attract to chemical synthesis the most capable young people. The

unpleasant situation presently noted by virtually all VUZ instructors is that the chemical student body has demonstrated loss of interest in substances and, consequently, in synthetic work, i.e., the essence of chemistry. Most talent students presently prefer to work with instruments, computer methods and monitoring methods.

To what can we attribute the diminished interest of young people in synthesis? Of course, the unique attraction of instrument and computer equipment is felt here. However, this is still not the main factor. One should consider the overload of students with mandatory disciplines to be a very relevant factor: little free time remains, and the student strives to use it in such a manner as to obtain as quickly as possible data needed to speak at a scientific conference or prepare a publication. These requirements are met quite satisfactorily by making measurements with instruments of the properties of known compounds or evaluating these properties by means of mathematical calculations.

The first positive results in synthesis work come much later. This is attributable to the longer acquisition of experimental skills and specifics of organic synthesis: here, experiments last for a long time, they often end in failure, they must be repeated many times, which requires exceptional patience. It is apparent that, when time is short, the new student could give up after the very first failure. Here, a scientific supervisor could be helpful, but instructors are also overloaded with their teaching work, they are physically incapable of devoting the required time to students interested in synthesis.

Finally, the last and probably main reason for departure of young people from organic synthesis is, as we have already discussed, the extremely poor equipment of the vast majority of VUZ laboratories. When there is a chronic shortage of good glassware, equipment and reagents, an experiment sometimes becomes a torment; as a result, the students have to synthesize the most elementary substances, and in essence they are faced with yesterday's tasks. As a result, the young specialist gradually develops a psychological barrier, a sort of allergy to complicated research.

This, in turn, hinders development of another very important trait of the synthetic chemists, the ability to make up a plan for complex organic synthesis. Alas, not only students, but many experienced specialists in synthesis are wanting in this ability.

#### Organization of Work

Solution of the problems with reagents, equipment and personnel training will not yield the expected results if a mechanism is not created to assure good organization of labor for synthetic chemists and their orientation toward solving major problems. If, for example, we were to ask ourselves: "What forms of scientific research do we need to work on synthesis of dodecahedrane?" it would lead us to a dead end. And this is not surprising, since such work requires considerable time, an impressive staff of strong executors and considerable risk: what if nothing is achieved? Especially, since it is difficult to expect a direct practical benefit from dodecahedrane itself.



We have virtually no forms for such expenditures, and this is a bad thing, since many valuable synthetic ideas remain unrealized. Graduate student programs, cost-accounting work, research within the framework of various assignments according to plans--each of these forms of organization of scientific research has proven its usefulness and viability. But they do not cover the entire spectrum of needed activity, namely the part that is needed to perform tasks at the leading edge of organic synthesis.

I am convinced that we must adopt the knowhow of all industrially developed countries where a substantial if not main part of pioneering research has, for a long time, been done by postdoctoral fellows (doctors of sciences--the equivalent of our degree of candidate of sciences). Such fellowships are offered soon after defending a dissertation; at their own choice or upon receipt of an invitation, the fellows (and often the demand for them exceeds the supply) are assigned to work with some professor who has a fruitfully functioning scientific school. These professors, in turn, are allocated special funds for scientific research, including stipends.

Students, graduate students and young members of the department staff converge around the fellows, and a team is formed that has a very valuable set of qualities: high qualifications of most executors, who also have a fair amount of ambition, the opportunity for exchange of knowhow among team members and constant influx of fresh recruits. It is expressly in such teams that new ideas are tested.

Under the conditions prevailing in our country, it would be wise to establish, at first, several dozen such funds, granting the right to use them, perhaps, primarily to professors at the major VUZ's known in scientific circles for their achievements and interesting ideas. It would be reasonable to allocate funds for 5-6-year periods and extend them only if the team achieves outstanding results.

Confusion and lack of system are contraindicated for organic synthesis. Here, an environment of free search and liberty are important to fruitful work. For this reason, one should relieve creative teams of petty patronage, rigid planning, and reduce to a minimum intermittent reporting. There are quite a few objective criteria of a high quality of scientific research.

The question may arise as to what should be done about introduction of obtained results to practice. The answer is as follows. In the first place, we have been dealing in this article with providing optimum conditions for development of basic research. Work of an applied nature could develop independently, but there is no doubt that the proposed measures will have the best effect on it. In the second place, experience has shown that, sooner or later, the results of basic research will make their way in life where its level is high. Finally, the emergence in our country of numerous highly qualified synthetic chemists capable of tackling any extremely complex problem must be worth something.

Thus, let us sum up. Fine organic synthesis requires urgent help and attention. The steps that will have to be taken for this will require serious restructuring, abandonment of many customary stereotypes. It is deemed

mandatory, for the purpose of itemizing a program for development of organic synthesis in our country, to establish an interagency committee, which would have the appropriate authority, including representatives of the State Committee for Science and Technology, USSR Ministry of the Chemical Industry, Academy of Sciences and USSR Ministry of VUZ. Apparently, a representative of GKNT should head such a committee, since all of the planned measures should be viewed as an element of the "Combined Program for Use of Chemistry in the National Economy of the USSR for the Period up to the Year 2000."

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ECONOMETRICS AND COMPUTERIZED DATA PROCESSING IN PLANNED EXPANSION  
OF CHEMICAL INDUSTRY

Moscow KHIMICHESKAYA PROMYSHLENNOST in Russian No 3, Mar 87, pp 186-189

[Article by R. D. Ivleva, N. A. Kryukov, L. S. Presman and I. V. Sheynina  
(deceased)]

[Abstract] A survey was conducted on the current needs for the further developments of the Soviet chemical industry, based on the requirements for a balanced economic growth of the USSR as postulated in resolutions of the 27th Party Congress. It is evident that econometrics must be employed in any assessment of the current status of the chemical industry to derive a solid foundation for planned advancements, as well as in formulating plans for further expansion of this particular sector. To date, however, econometrics have received largely a philosophical recognition, and the immediate needs are for the actual implementation. It has been further recognized that computer-based data processing provides the key for the management of statistical and economic data, and for ensuring operational efficiency via expansion of automation at the work site. The combination of an econometric approach and computerized data processing can, and will, make the difference in any attempts at improving labor productivity and the cost effectiveness picture. Tables 1.

12172/5915  
CSO: 1841/293

LASER ACADEMY OF SCIENCES AND ESTABLISHMENT OF CHEMICAL SCIENTIFIC  
PRODUCTION COMPLEX IN OLAYNE

Riga IZVESTIYA AKADEMII NAUK LATVIYSKOY SSR in Russian No 11, Nov '86  
(manuscript received 5 Mar 86) pp 36-44

[Article by M. V. Shimanskaya and Ya. P. Stradyn, Institute of Organic  
Synthesis, LaSSR Academy of Sciences]

[Abstract] The authors summarize the history of the formation of the precision chemical production complex at Olayne, near Riga. The Scientific Production Association "Biolar" and the "Olaynfarm" Production Association cooperate closely in production of organic chemical products and pharmaceuticals. The

lack of natural resources in Latvia is balanced by a long history of chemical production going back to 1862, while the various institutes of the Latvian Academy of Sciences have invented and developed numerous marketable compounds, including purines, pyrimidines, nucleosides and nucleotides, DNAs and various enzymes. Antibiotic production after 1945 and development of pharmacopoeia data are summarized. Factors leading to construction of this advanced chemical and pharmaceutical complex and the course of construction are outlined. In order to generate scientific contacts and exchange of information and licenses, scientific conferences have been organized at the facilities, beginning in 1963. Plant officials have traveled around the Soviet Union and to Hungary to learn modern production procedures. In addition, the needs of modern chemical and pharmaceutical production led to the establishment of specialized institutes to develop needed technology. The work of G. A. Giller and his collaborators in the Institute of Organic Synthesis of the Academy have been instrumental in the progress of the Olayne complex. The "Olaynfarm" Production Association has a special interest in nitrofuran preparations for health and animal husbandry. References 17: 16 Russian, 1 Latvian.

12131/5915

CSO: 1841/260

SUCSESSES AND PROBLEMS OF 'MEMBRANY' MNTK

Moscow SOTSIALISTICHESKAYA INDUSTRIYA in Russian 29 Apr 87 pp 1-2

[Article by Ye. Leontyeva, deputy newspaper editor, Science and Technical Progress Department, under rubric "How Are Things Going at the MNTK [Interbranch Scientific-Technical Complex]?": "In Search of a Consumer"; first two paragraphs are source introduction]

[Text] Membrane technologies are bringing the national economy revolutionary changes -- that is already axiomatic. Their "distinguishing features" are their low energy consumption and high economic efficiency, simplicity, accessibility, and their ecological efficiency. With their help it is possible to preserve fetuses and obtain valuable protein products from serum, to purify runoff water and gas effluent, to sterilize juices, and to perform a large number of other operations.

It would seem that the economic managers should literally "dig out" unique membrane sieves from one another. However, they are maintaining surprising calm, and, incidentally, there are reasons for this.

We are far from the first to produce membranes. This year, if we hurry, we shall reduce the lag behind world production to one-tenth. Last year the gap was more threatening.

And we are not the pioneers in this area -- scientists in California began to use a polymer sieve to freshen water as long ago as the 1960's. There is a certain element of lack of planning in the fact that at the present time we are already using them in a few places. True, developments have already been in progress for a long time at a number of institutes, but in an uncoordinated and sluggish manner. Most often, they are based on personal initiative and enthusiasm.

"Yes, we were not at a high level," V. Dubyaga, deputy general director of the Membrany Interbranch Scientific-Technical Complex [MNTK], says.

It is obvious that they were not at a high level, although it was specifically the Vladimir VNIISS [All-Union Scientific Research Institute of Arid Subtropics], which currently has become the nucleus of that complex, that engaged in that very promising process earlier than everyone else (starting in

1977) and more than the others. For this we thank them. As for scientific foresight, the analysis of worldwide practice and realistic forecasts, without which the planning of new technologies in the branch would be unthinkable, neither the developers nor the Minkhimprom [Ministry of the Chemical Industry] specialists and administrators had any of them. Hence the "tailism."

But then, starting in 1985 -- after two USSR Council of Ministers decrees -- the slightly delayed membrane boom started. It was then that the interbranch complex was formed, a complex which was called upon, within the shortest period of time, to bring revolutionary innovation up to advanced worldwide limits. The makeup of the newborn MNTK included at first seven production and scientific-production associations, as well as rather solid scientific-research and design subdivisions. In addition, about 20 organizations and enterprises were also switched in, which are not part of the complex but which are called participants in it.

And now a few figures. In the present year the lead organization of the MNTK (the Polimersintez Scientific-Production Association) is supposed to produce 32,000 square meters of membranes. But the confirmed need for them -- that is, production orders with a guarantee of payment -- exists for only one-third of the planned output. The administrators of the complex are greatly concerned by this. Of course, they are undertaking efforts to catch unenlightened economic managers on the hook of new technical decisions -- they are sending out letters and advertising prospectuses. It might be that some people are already "pecking" at them. But the worries are serious ones: the lead organization is capable of fulfilling the plan, but a considerable part of the output will have to be put into the warehouse. And, as the economists say, this is frozen capital.

You will agree that the present-day correlation between production and demand did not just come from thin air. It was previously influenced by our truly astonishing incompetence in questions of developing a world market. And if the market caught even scientific researchers unawares, what can one expect of the consumer who is completely accustomed to traditional technologies? Just think about how to shake him up and make him an active customer. This is now one of the chief tasks of the MTNK, inasmuch as it has been made responsible not only for developing and producing membranes, but also for using them.

In order to implement that task, the complex needs freedom to maneuver. It is necessary to have time to arrange reliable interrelationships with the consumers. And that must be done right now, inasmuch as the plans for the current five-year plan include the benefit from using membrane technologies with a value of 800 million rubles. For purposes of comparison, in the last five-year plan it came to 27 million.

"Just the same, you won't go far on advertising, information, and letters," MNTK director L. Pokrovskiy says. "What is needed here is a fundamental decision. Namely, to convert the MNTK into a company that provides the output on a turnkey basis."

Actually, how frequently do we abuse enterprise managers because they turn away from the new technology and technological schemes offered to them. It is

an understandable situation -- most frequently these innovations mean for the manager only confusion that is not compensated for by any of the subsequent results. He will give more reasons against this than you have fingers: the deliveries are made without components, they are not made on time, the process is not completely worked out, we don't have the proper personnel, etc. But why, then, is it that not a single enterprise refuses imported technology? Is the quality better? Not always. The plant gates are opened to it chiefly because of the service provided. The company officials deliver the equipment promptly and with all the components. And they adjust it and start it up. And they also teach people how to handle it.

Putting it more briefly, this is a matter of the efficiency of introducing innovations as the chief factor in attracting the consumer. Can the MNTK guarantee this? Not yet, but in any event it is already trying. Special mobile units can be seen traveling along the oblast roads, going from one enterprise to another. The chemists, for example, visited a machine-building enterprise where, after painting, a large quantity of paint and lacquer materials are discarded. They showed how to extract those discarded products from the runoff and return them to production. The annual benefit is 1430 rubles per square meter of membrane surface. And there is considerable benefit to the environment. They went to a dairy plant, and engaged in agitation work again. The ice started to break up. And already the people in Leningrad and Minsk and in Odessa and Arkhangelsk are beginning to invite the people of Vladimir to visit them.

But there are only two units -- in general, a miserly amount. In addition, there are not enough trucks to transport them, and there is a gasoline shortage. Let us assume that we have found both the trucks and the gasoline. We have loaded the unit, taken it to Leningrad, unloaded it there, and, naturally, have sent the truck back to Vladimir. There another customer gets in touch with them -- and he is in Gorkiy. The people at Vladimir tell him to take his truck and drive it to Leningrad. And the customer with a truck and gasoline is also in an awkward situation. Meanwhile, the nomadic unit, as a result of being loaded and unloaded numerous times into and out of the truck body, and as a result of the lack of careful hands, gives up and refuses to operate. That's what all the service gets you!

What are people at VNIISS dreaming about? About the most vital thing at the given moment: getting vans that can be used only for purposes of serving the customers and for no other purpose. They are dreaming of installing the units in them permanently, and giving each unit a personal operator. And of offering their services, as the expression goes, with home delivery and in complete volume. If, after seeing the commodity face-to-face, the customer is interested, then it is possible to weigh its capabilities and determine its necessary size. Then you can go on and prepare the production area and we will bring you the required technology, adjust it, bring it up to the proper parameters, and turn it over to you on a turnkey basis.

When will the dream become reality? By the end of the five-year plan, the MNTK managers assert. But there are many things that have to be done by that date, which really is not too far away. The pool of mobile vehicles does not yet exist -- it is hoped that they will be received within the next two

years. The units are not particularly what we want. They lack modern automatic equipment and means of control. A state-of-the-art base for testing and manufacturing them is needed. But VNIISS has only machine shops, and nothing more. A specialized shop is needed. Without it, it is currently as though there were no hands there. When will it be ready? No sooner than 1990.

Things are going slowly. But the opportunities for accelerating the situation probably do exist. A discussion that I had with the complex managers centered basically on the needs and capabilities of the lead organization. The impression was formed that it is still difficult for them to become aware of the fact that they have tremendous opportunities in their hands. I have in mind the potential and resources of the MNTK participants. One has machine-building capabilities, another has an experimental base, a third has test stands, and a fourth has electronics. And so on. It is, of course, no simple matter to collect all these opportunities into a single fist. But one must engage in these matters constantly, daily. For example, every participant has his own tasks, which are set forth in the branch programs that have been computed until the year 1990. Ideally, one should currently keep them constantly in one's sight, but at the lead organization the file containing these programs is not yet full. One contracting party acts in a leisurely way, engaging in things in the customary way, "like our department does it," and another contracting party also is in no hurry. As a result, there is no common cause.

It turns out that the participants are structurally united, but are not yet strongly linked by their common tasks. One could convoke an MNTK council, but that too would be a problem. In response to the invitation to come to a session of it, one can hear the reply: first get us an authorization from the ministry leadership to make the trip... The MNTK partners have brought their departmental habits into the interdepartmental organization. Overcoming them is important work on the path to the consumer who, as yet, is not interested.

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UDC 541.49:541.128+541.182:546.98

## FROM POLYNUCLEAR COMPLEXES TO COLLOIDAL METALS

Moscow ZHURNAL VSESOYUZNOGO KHIMICHESKOGO OBSHCHESTVA IM. D. I. MENDELEYEVA  
in Russian Vol 32, No 1, Jan-Feb 87 pp 36-42

[Article by M. N. Vargaftik, candidate of chemical sciences, Institute of  
General and Inorganic Chemistry imeni N. S. Kurnakov, USSR Academy of Sciences]

[Abstract] The analysis of metallic clusters such as thin films and deposited heterogeneous catalysts is difficult in terms of traditional coordination chemistry. The study of oxidative changes in unsaturated compounds catalyzed by Pd complexes provides one approach to understanding the nature of cluster particles and metal complexes containing transition metals. Ethylene oxidation can be catalyzed by  $\text{Pd}^{\text{II}}$  in 1-, 2-, or 3-nuclear complexes without metal-metal bonds, with the resulting product also obtainable with a catalyst of Pd on an inert substrate. However, for higher olefins and aromatic compounds, heterogeneous catalysts generally result in different products, probably through catalysis by  $\text{Pd}^0$  or  $\text{Pd}^{\text{I}}$ . Stable polyhedral complexes of  $\text{Pd}^{\text{I}}$  can be formed by oxidation of carbonylphosphines of  $\text{Pd}^0$  or reduction of  $\text{Pd}^{\text{II}}$  complexes, although these are easily poisoned by CO. Oxidation of propylene or toluene can be catalyzed by more stable Pd clusters formed with carbonylphosphine ligands in 1,10-phenanthroline or 2,2'-dipyridyl and having a nominal degree of oxidation of the Pd of +0.3. These noncrystalline clusters apparently have a nearly spherical metallic lattice with regular dispersion of the metal atoms and a particle size of approximately 25 Å. Inter-atom distances indicate that packing of the metal atoms is in the form of a multilayered regular icosahedron. Such icosahedral clusters can contain 13, 55, 147, 309, 561 etc., metal atoms; other clusters with 55 metal atoms are known, but their geometry is still uncertain. However, they typically have a central metallic core surrounded by a layer of ligands. The Pd cluster has a similar structure; experimental data indicates a 5-layer icosahedral structure with 561 Pd atoms, apparently with 60 coordinating ligand groups and 180 acetyl groups. In this arrangement, most surface atoms of Pd are sterically hindered from acting catalytically; oxidative-reduction processes probably take place by electron transfer through the metal skeleton. Larger yet are mycelles of hydro- or organosols of metals, usually formed by reduction of ligand complexes of metals such as Au. This involves two competing processes--the formation of a metallic lattice and the coordination of ligands with metal atoms on the surface of the cluster. The ligand envelope may also include molecules of a solvent, as with toluene in a  $\text{Co}^{\text{II}}$  complex. Apparently, initial metal lattices often differ from the typical

lattice of the bulk metal, particularly when formed from the gas phase on solid substrates. For such small clusters, stabilization can be supported by partial dispersion of the normal electron density away from the metal lattice, with negatively charged ligands on the outer surface. While molecular clusters have a discrete molecular mass and an exact chemical composition, colloidal clusters are characterized by a dispersion in both size and exact chemical composition. Figures 6; references 66: 29 Russian, 37 Western.

12672/5915  
CSO: 1841/274

UDC 535.17

OPTICAL PROPERTIES OF CLUSTERS OF COLLOIDAL PARTICLES OF SODIUM IN  
CRYSTALLINE NaCl

Riga IZVESTIYA AKADEMII NAUK LATVIYSKOY SSR in Russian No 1, Jan 87  
(manuscript received 26 Nov 86) pp 102-111

[Article by Ya. A. Ekmanis, I. S. Radchenko, V. M. Bezruchko and K. K. Shvarts; Institute of Physics, LaSSR Academy of Sciences; Krivorog Mining Institute; Kiev State University imeni T. G. Shevchenko]

[Abstract] Heterogeneous dispersion of colloidal Na particles by volume and size can significantly affect the optical properties of crystalline NaCl. However, calculated values of the attenuation coefficient of optical illumination and associated parameters differed by two orders of magnitude from experimental values, probably due to: the microcharacteristics of colloidal Na differing from that of bulk Na, the presence of liquid Na particles (above 370° K), nonspherical particles, and clustered, rather than evenly distributed particles. Calculations indicate that the coefficient of attenuation decreases for particles of size 20-30 nm and is substantially affected by the degree of oblateness of spheroidal particles. Shifts of the band of attenuation of colloidal particles on heating is less than what can be attributed to a simple transition to a liquid phase; this is apparently due to a combination of increased particle size with an associated rise in hydrostatic pressure and change in the melting point of the colloidal Na. Clustering of particles in chains or spherical groupings also changes the optical parameters when the distance between individual particles is less than four times their radius. This is due to the shielding of inner particles from electromagnetic waves, with chains of spherical particles acting analogously to spheroidal particles. Taking the calculated values of these four effects into account and assuming a logarithmic size distribution of Na particles produced a theoretical curve of the spectral dependence of the coefficient of attenuation of optical illumination in the NaCl-Na system which was in close agreement with experimental data. Figures 7; references 21: 6 Russian, 15 Western (3 by Soviet authors)

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CSO: 1841/269

UDC 541.095

## EXPLOSIVE CHEMICAL REACTIONS IN SOLIDS

Moscow DOKLADY AKADEMII NAUK SSSR in Russian Vol 292, No 5, Feb 87  
(manuscript received 22 Sep 86) pp 1165-1169

[Article by Academician N. S. Yenikolpyan, V. B. Volyeva, A. A. Khzardzhyan and V. V. Yershov, Institute of Synthetic Polymer Material, USSR Academy of Sciences; Institute of Chemical Physics, USSR Academy of Sciences, Moscow]

[Abstract] A study is reported of exothermic chemical reactions occurring in solids during an explosion. The experimental installation used a Bridgeman anvil and extrusion of solid substances through a cone. Analysis of the reaction products was by two methods: gravimetric analysis and infrared spectrometry. Calculations showed that the energy necessary to disperse the initial particles as observed was an order of magnitude higher than the mechanical energy in the system. However, in addition to the mechanical energy of compression, there is another source of energy--the heat of reaction--which provides sufficient energy for mass transfer at the molecular level. However, since in order for the reaction to occur additional energy must be supplied, while the additional energy can be obtained only by the reaction itself, it is obvious that the process does not occur simultaneously in the entire volume of the specimen tablet, but rather in stages at the reaction wave front, with each layer in which the reaction has occurred providing energy for continuation of the reaction in the next layer. The wave-front of propagation of the process through the tablet begins at the periphery, not at the center. Figures 2; references 10: 9 Russian, 1 Western.

6508/5915  
CSO: 1841/297

UDC 541.136.52

## BEHAVIOR OF IN-AIR HYDROPHOBIC ELECTRODES AT ELEVATED TEMPERATURES

Kiev UKRAINSKIY KHIMICHESKIY ZHURNAL in Russian Vol 53, No 2, Feb 87  
(manuscript received 23 Jul 85) pp 174-177

[Article by S. N. Kravchenko, A. M. Trunov, Ye. U. Labkov, A. A. Dzhambek  
and N. N. Verenikina, Odessa University; Odessa Naval Engineering Institute]

[Abstract] The authors report on development of an electrode system with more durable microstructure based on an innovative, gas conducting film that makes possible observation of temperature values without prior temperature preparation. Fine-structured nickel was used as the base upon which an electrocatalytic active layer, consisting of a nickel cobalt spinel with a fluoroplastic component, was pressed at 150-190 kg/cm<sup>2</sup>. The electrodes, with working surfaces of 2.5 cm<sup>2</sup>, were then tested in a KOH solution; they were compared to mercury oxide electrodes. An exponential dependency of current on potential was established by a regression method. Analysis of data indicate that with less than 20% oxygen in a gaseous mixture and at ca. 30 millamperes/cm<sup>2</sup>, the tested hydrophobic electrodes showed a transition to extreme current zones, with a nearly proportional dependency of current on oxygen content. Two mechanisms for generating current in gas-diffusion electrodes are related to the catalyst at low concentrations and, most importantly, to the electrical conductivity of the electrolyte in the active layer, gas solubility in the electrolyte, diffusion coefficients of gas and ions and film parameters. Polarizing resistance was found to be useful as a general parameter; the lower its value the more intensive the current formation process. Activation of ohm-diffusion resistance was reduced when oxygen instead of air was supplied to the process. Further refining of the microstructure of the tested electrode should intensify the process of electrical reduction of oxygen. References: 11 Russian.

12131/5915  
CSO: 1841/280

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PROGRAMMING ENVIRONMENTAL PROTECTION RESEARCH IN CHEMICAL INDUSTRY

Moscow KHIMICHESKAYA PROMYSHLENNOST in Russian No 3, Mar 87 pp 179-182

[Article by A. V. Putilov]

[Abstract] Spatial programming is being advanced as an optimum approach to fundamental research on environmental protection in the case of the chemical industry, designed to minimize and eliminate common causes of pollution. The different phases of a multifaceted program have been designed in the form of a three-dimensional model, accommodating physicochemical methods in the form of trajectories applicable to different aspects of the pollution problem. The three-dimensional construct facilitates identification of the best methods to manage a pollution problem via delineation of the desired end effects in conjunction with assessment of economic impact and technological feasibility. The programming approach may be used as a working instrument in the management of scientific and technological advancements vis-a-vis environmental protection. Figures 3; references 10: 9 Russian, 1 Western.

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BEHAVIOR OF  $^{238}\text{U}$  and  $^{232}\text{Th}$  IN SOILS OF CENTRAL ASIA

Moscow AGROKHIMIYA in Russian No 3, Mar 87 (manuscript received 25 Apr 86) pp 83-86

[Article by G. S. Ishchenko, A. S. Butnik, T. F. Afanasyeva, V. A. Rastopchina and Z. G. Ovchinnikova, Central Asian Scientific Research Institute of Phytopathology, Tashkent]

[Abstract] Laboratory experiments on the adsorption processes and forms in which  $^{238}\text{U}$  and  $^{232}\text{Th}$  were present in soils were undertaken to determine the influence of soil properties on the behavior of the nuclides. Five soil types were used, differing in content of humus, physical clay and minerals. The degree of fixation of  $^{238}\text{U}$  was found to vary with the physical and chemical

properties of the soil. The greatest quantity was adsorbed by meadow and swamp soils with high content of humus, physical clay, potassium and calcium.

$^{238}\text{Th}$  was adsorbed completely by all soils. Uranium and thorium are extracted from the soils by various desorbents from 0.5-35.9% to 0.08-20.4%. The best extracting agent for uranium is ammonium carbonate, for thorium--calcium chloride solution. An inverse correlation is observed between the content of more mobile forms of uranium and thorium and the content of physical clay humus, potassium and calcium in the soil. References: 5 Russian.

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UDC 628.162.534+576.858.9+661.184.23

#### INTERACTION OF VIRUSES WITH MONTMORILLONITE

Kiev KHIMIYA I TEKHNLOGIYA VODY in Russian Vol 9, No 1, Jan-Feb 87  
(manuscript received 11 Mar 85) pp 19-22

[Article by L. I. Globa, G. N. Nikovskaya, Yu. I. Tarasevich, Institute of Colloid Chemistry and Water Chemistry imeni A. V. Dumanskiy, Ukrainian Academy of Sciences, Kiev]

[Abstract] A study was made of the influence of virus dimensions, pH and salt composition of an aqueous medium on the effectiveness of adsorption of viruses by montmorillonite particles. E. coli phage T2 and E. coli phage MS2 K-12 were used as the model viruses. The interaction of the viruses with the clay mineral was found to be electrostatic in nature. Large viruses were adsorbed in macropores of the adsorbent, while the smaller viruses probably reached the well-developed mesopore space. The large viruses had greater affinity for the adsorbent than the smaller ones. Interaction of the viruses with the montmorillonite can be described from the standpoint of heterocoagulation-heteroadagulation theory, and also by an adsorption approach. Montmorillonite is promising for water purification, providing rapid and effective adsorption of viruses in the processes of coagulation, sedimentation and filtration. Figures 3, references 10: 8 Russian, 2 Western.

6508/5915

CSO: 1841/307

## RADIATION-ADSORPTION PURIFICATION OF WASTE WATER CONTAINING PESTICIDES

Kiev KHIMIYA I TEKHNLOGIYA VODY in Russian Vol 9, No 1, Jan-Feb 87  
(manuscript received 21 Mar 85) pp 68-70

[Article by G. K. Nikonorova, S. A. Brusentseva, V. N. Shubin, D. M. Zorin, A. A. Sosnovskaya, Ye. P. Petryayev, V. I. Vlasova, I. P. Yedimecheva and N. N. Subbotina, Institute of Electrochemistry imeni A. N. Frumkin, USSR Academy of Sciences, Moscow; Belorussian University, Minsk]

[Abstract] Radiation-adsorption purification of water combines adsorption purification with simultaneous irradiation of the adsorbent, increasing the protective life of the adsorbent by radiation regeneration of charcoal. The method can be used to remove pesticides such as 4,4-dichlorodiphenyltrichloroethane (DDT),  $\gamma$ -hexachlorocyclohexane (HCH), dimethyl-2, 2-dichlorovinylphosphate (DDVP) and petroleum products. Utilization of continuous irradiation of an activated charcoal layer was found to increase the protective life of the adsorbent from 93 to 156 days. Lower radiation doses are required when radiation alone is used, and consumption of activated charcoal is reduced. Figure 1; references: 11 Russian.

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CSO: 1841/307

## DISTRIBUTION OF PLUTONIUM AMONG COMPONENTS IN NATURAL ORGANIC SUBSTANCES AND THEIR ROLE IN ITS MIGRATION IN SOILS

Leningrad RADIOKHIMIYA in Russian Vol 29, No 1, Jan-Feb 87  
(manuscript received 21 Apr 86) pp 99-106

[Article by F. I. Pavlotskaya and T. A. Goryachenkova]

[Abstract] The purpose of this work was to study the bonding of plutonium with individual components of organic matter in various types of soil and their role in its migration in the soils. Typical forest and forested-steppe soils were studied, contaminated with plutonium under laboratory conditions and held air-dry for 3 years. The plutonium was found to be bonded with practically all groups of soil organic matter. The plutonium content and humic acids increased in the sequence: Soddy-podzolic < grey < chernozem, which correlated with their content of organic carbon. The contents of plutonium and the individual organic components plus data from earlier studies on extractability of plutonium from various soils by alkaline solutions and absorption with humic acids indicate that the plutonium is present in the soils in various compounds. The predominant mechanism of slow transfer is migration of plutonium as finely dispersed particles as the soils are washed by

precipitation. Rapid transfer results from migration of soluble complex compounds of iron and aluminum with acids. The migration capability of plutonium falls in the following sequence: Soddy-podzolic > grey forest soil > chernozem. Plutonium is primarily carried with various compounds of calcium, iron and aluminum, which determine its migration in soils. References 28: 15 Russian, 13 Western.

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UDC 546.79:541.183.24+551.464

#### ADSORPTION OF CESIUM FROM SEA WATER SOLUTIONS

Leningrad RADIOKHIMIYA in Russian Vol 29, No 1, Jan-Feb 87  
(manuscript received 8 Sep 85; in final form 1 Oct 86) pp 127-129

[Article by N. D. Betenekov, V. V. Kaftaylov and I. Ye. Bushkov]

[Abstract] The long-lived radioactive isotopes  $^{90}\text{Sr}$  and  $^{137}\text{Cs}$  make the major contribution to global radioactivity of the seas and oceans resulting from human activity. This article presents experimental data on adsorption concentration of  $^{137}\text{Cs}$  from imitation sea water by means of a thin layer potassium-iron hexacyanoferrate sorbent obtained by precipitation of iron hydroxide onto the surface of cellulose with subsequent modification of the hydroxide to hexacyanoferrate. The adsorption of cesium was found to follow Henry's rule, the rate of adsorption being limited by external diffusion. The distribution coefficients determined by static and dynamic experimentation agreed within the limits of experimental error. A significantly higher rate constant was obtained under dynamic conditions than in a limited volume study, possibly a result of better hydrodynamics of the flow of the solution around adsorbent grains and the higher m/V ratio. Figures 2; references: 9 Russian.

6508/5915  
CSO: 1841/300



## NEW TECHNOLOGY IN FERTILIZER INDUSTRY

Moscow SOTSIALISTICHESKAYA INDUSTRIYA in Russian 29 Apr 87 p 2

[Article by G. Sergeychuk, chief agronomist, Fertilizer Quality Inspectorate, USSR Gosagropom, and S. Sakhno, TASS correspondent, Moscow, under rubric "Action by SOTSIALISTICHESKAYA INDUSTRIYA and TASS: From the Institute to the Field": "'Someone Else's' Trouble"; first paragraph is source introduction]

[Text] With sledgehammers in their hands, the farmers approach the output that has been developed by the leading institute of USSR Minudobreniy [Ministry of Mineral Fertilizer Production] -- NIUIF [Scientific Research Institute of Fertilizers, Insecticides, and Fungicides] -- in Doctor of Technical Sciences A. Kononov's laboratory. This is the only way the monolith that the nitrofoska [nitrogen-phosphorus-potassium fertilizer] has become can be prepared for field operations. The nitrofoska has come from the laboratories of that honored institution and is produced in tremendous quantities by the Azot Associations in Ionava and Novgorod, as well as by the Dorogobuzh Nitrogen Fertilizers Plant. After two or three months of storage, that output becomes almost unsuitable for agricultural purposes. But the suppliers will not furnish any other fertilizers: use what you've received, is the answer they give.

And it is difficult to reproach them: according to all the approved documents, the scientists and production workers guarantee the quality of this type of fertilizer only at the moment that it is turned over to the customer. As for what happens after that, it's not their worry.

Could it be that "fresh" nitrofoska is good? Yes, one can actually deal with it without using a sledgehammer. At the warehouse of the Vasinskiy Sovkhoz in Smolensk, two women with sieves sift and package into sacks the fertilizers that have just been produced and which have already had time to cake. We saw the same picture, with the same "progressive technology," at other farms in this oblast. The situation is no better in other locations. The farmers in Voronezh, for example, knowing these properties of the fertilizers, have previously laid in a supply of 2 million sacks to package the output. It would seem that it would be simpler to do that at the plant. But the GOST [All-Union State Standard] that regulates the shipment conditions stipulates two alternatives: either in packaging, or without it. And so the enterprise chooses what is simpler and cheaper, and it is the kolkhoz members who get the

extra trouble, expenditures, and losses.

The roots of these problems go back to the laboratories and administrative offices of the Scientific Research Institute for Fertilizers, Insecticides, and Fungicides imeni Professor Ya. V. Samoylov (NIUIF) (director, A. Novikov; partkom secretary, V. Tersin). At one time this institute created a rather large number of innovations that farmers needed. One still encounters such truly high-grade fertility stimulators. For example, the diamoniyfosfat [diammonium hydrogen phosphate] produced by the Azot Association in Cherepovets.

But the topic of discussion is not the merits of the decorated collective -- they only confirm that outstanding output can also be produced here. But why? Because no one is held responsible for a bad development and a bonus might even be paid for it as an innovation.

Quite recently the Azot Association in Nevinnomyssk used to produce, in series production and with impunity, nitroammosfos [nitrogen ammonium phosphate], which also had the property of very rapidly converting into a monolithic mass. In many parts of the country it formed indestructible monuments to the inefficiency of the scientists and production workers. After many complaints, indignant letters, commissions, and sessions, the production of the "fertility stone" was discontinued. Instead, the scientists proposed to the association that it produce liquid combined fertilizers. Apparently, there was the hope that at least they would not harden. The scientific forecasts were not justified: at positive temperatures, active crystallization immediately begins. But the enterprise stubbornly continued to provide the farmers with this effective "innovation."

However patient the representatives of USSR Gosagroprom are, even they finally gave up: they levied a fine of more than 3 million rubles on the association. An interesting position in this story was occupied by the party's Stavropol Kray Committee, which rose in the active defense of the producers of the defective fertilizer. And again NIUIF was not involved. The people there were calmly and knowledgeably preparing for the certification of their latest development for the Quality Seal.

This aspect of the institute's activity is of no small importance. After they began to be fined for Category I, a real battle for the Quality Seal broke out. But that battle is raging not in scientific laboratories or in production, but in the offices of USSR Gosagroprom, where scientists headed by deputy director of NIUIF, F. Yanishevskiy, with the support of the ministry, and with energy that is worthy of better application, are literally "punching" a way for their developments. All things considered, they have achieved a definite success, because a number of fertilizers about which the farmers are actively complaining continue to be given the honored pentagon.

When submitting output for the Quality Seal, it is necessary to indicate foreign counterparts (the article must conform to the world level). By taking advantage of the poorly organized scientific-technical information service with regard to this question, the interested party takes the most convenient and the oldest counterparts. One of the fertilizers even has a 1973

counterpart. The least authoritative companies are taken as a guide. All this makes it possible to delay bringing the development up to "worldwide models."

In addition, the pedestal of the highest category is easily accessible also because of the imprecision of the standards that have been established for many fertilizers. Take, for example, GOST 2081-75 for carbamide. That standard specifies strict parameters for that product. But it immediately stipulates, in a footnote, the possibility of the nonfulfillment of the basic parameter. Many other GOST's have also become "flexible" -- being altered in the direction of reducing exigency with regard to quality.

This is the result of the lack of principles as demonstrated by Gosagroprom and Gosstandart and also the "merits" of the scientists, because, in a solid alliance with the Ministry for the Production of Mineral Fertilizers, they have been overcoming even other complications. Nevertheless, at one time Gosstandart demonstrated firmness and, by its 15 August 1985 decree, banned the production of ungranulated phosphorous fertilizers that do not conform to modern requirements. However, with the consent of USSR Gosplan, they continue to produce them to this day. True, it is with the stipulation that all of this is for industrial purposes. The Krasnodar Chemical Plant manufactures them for fodder additives. But the farmers, to whom the NIUIF scientists and the production managers have not yet provided a proper replacement, have been forced to continue using powder: fertilizers of this type are chronically unavailable, and for this spring alone deliveries of phosphorous dressings to farmers have been 2 million tons short. The strict ban has remained only on paper.

Of course, many of the problems mentioned were caused by the complicated conditions in which NIUIF operates. These include a weak material-technical base, and insufficient financing. However, the chief factor, people at the institute feel, is the shortage of cadres. If all the specialists involved in attending conferences and in "punching" and "pushing" developments ahead were to be requalified and were to engage in real work in the laboratories, things would get moving. And things must get moving immediately -- that is the command of the times.

5075

CSO: 8144/3993

SCIENTIFIC PROGRESS IN AGRICULTURE

Moscow KHIMIYA V SELSKOM KHOZYAYSTVE in Russian No 2, Feb 87 pp 2-4

[Article by Sh. I. Litvak, candidate of agricultural sciences]

[Text] In developing the material and technical foundation for an agricultural complex, it is necessary to raise the effective use of the available production potential and concentrate the forces and means on those directions which ensure the highest output.

(From the resolution of the XXVII Session of the Communist Party of the Soviet Union based on the political teaching of the Central Committee, CPSU).

The state plan for economic and social development of the USSR for 1986-1990 and the period to 2000 provides for an increase in the effectiveness of the production potential of the agricultural complex--creation of conditions for stable management of agricultural farming based on intensification and promotion of scientific and technical progress.

In the promotion of agricultural production, a special place is assigned to chemicalization. By 1990, it is planned to raise the volume of supplies of mineral fertilizers for agriculture to 31.0 million tons as compared to 25.4 million tons in 1985, to increase the supply of lime materials, pesticides and fodder preservatives.

Efficient use of chemicals lowers the cost of agricultural products and strengthens the farming economy. According to the data of the department of economics of TsINA0, in one year of the 11th Five-Year Plan, the return for one ruble spent for applying mineral fertilizers was 2.55 rubles and for plant preservatives 4.81 rubles of production. However, when critically evaluating this complicated situation, it must be noted that the normal return from fertilization in main agricultural production has not yet been achieved. For sugar beets, it amounts to 74%, for potatoes--53% and for vegetables--38% of the standard.

Among the factors ensuring the stability of agricultural development and high effectiveness of fertilization, soil fertility plays an important role. At present, the agrochemical properties of the soil are far from optimal.

In many regions of the country it is noted that humus of the soil is decreasing: 36% of the arable land contains little phosphorus, 10%--potassium; 24% needs lime treatment. About 22.9 million hectares of pasture land need gypsum treatment and reclamation. In large areas, the production of high and stable crops is limited by deficiency of trace elements in the soil.

The resources of mineral fertilizers must be used efficiently everywhere. At present, about one billion tons of organic fertilizers are applied annually to the fields of collective and state farms, of which only 500 million tons are from manure and compost. On every farm work has to be organized so that the nutrient content in one ton of organic fertilizers be raised to 12 kg and the amount of weed seeds be decreased by a factor of 15-20. In order to secure total balance of humus in agriculture, the level of production and application of fertilizers has to be raised to 1.5 billion tons. This will permit getting, additionally, 45 million tons of agricultural products calculated for grain. The use of turf as fuel has to be eliminated and the production of sapropelite has to be expanded to the maximum. The areas enriched by planting legumes must be extended to 10 million hectares.

Measures taken to increase the output of organic fertilizers and the improvement of their quality will make it possible to increase the profit from the use of fertilizers by at least 15-20%.

A decisive factor in agricultural efficiency is lime treatment of acid soils. The acid reaction of the soil medium is the main reason for low yields and shortages of a large quantity of agricultural products. The problem of lime treatment is seriously aggravated by the use of physiologically-acid mineral fertilizers which leads to a sharp calcium depletion in the arable land horizon.

On the average, per year in the 11th Five-Year Plan, 7.4 million hectares were treated with 45.5 million tons of lime materials, which still did not compensate for the calcium and magnesium depletion of the soil. Therefore, the areas needing lime treatment did not decrease during the last 15 years, rather they increased: in the Volga-Vyatka and the North-Caucasian regions by 0.2% and in the central-chernozem regions by 8.5%.

To eliminate the excess acidity of the soil, the average yearly lime consumption in the country has to be raised to 13 million hectares by 1990. This will involve a shift to a scientifically substantiated 4-5-year cycle of lime treatment. The 12th Five-Year Plan, provides for complete elimination of the strongly acid soils, characterized by the lowest fertility. The Planning-Research Chemicalization Stations and the rayon "Selskhokhimiya" Association must pay special attention to proper selection of areas for priority lime treatment, to improving the accounting and to the quality of the lime application work.

An important measure for increasing the effectiveness of the chemicals is the use of trace fertilizers. Considerable work is being done with them in the Moscow Oblast. According to data of agrochemical studies, at present 52% of plowland contain an insufficient amount of boron, 88%--molybdenum, 95%--zinc,

78%--cobalt and 50%--copper. On the basis of this information, the Planning-Research Institutes of Chemicalization have determined the requirement for trace fertilization in the oblasts. The resulting data, together with the results of agrochemical studies of the soil, are then carried to the farmers for practical application.

In many regions of the country, there is sulfur deficiency. Therefore, the work program of the agrochemical service for the 12th Five-Year Plan foresees the completion of agrochemical assay of soil for sulfur content, the execution of field experiments with sulfurous fertilizers and the determination of the sulfur balance.

In searching for ways to restore soil fertility, effective application of fertilizers and other chemical agents, the agrochemical service began a complex agrochemical cultivation of the fields in 1981.

Systematic work for increasing the soil productivity is a key problem which determines the agricultural development especially in the non-chernozem zone. With broad agrochemical cultivation, grain output increases by 5-8 quintals per hectare, potatoes by 25-30 quintals/ha, and the green mass of annual cultures and corn by 45-50 quintals/ha. Substantial experience in experimental work in the complex agrochemical cultivation of the fields has been collected by the agrochemical service of the Russian Federation. Considering the existing phosphorus deficiency in agrochemical cultivation, phosphorite fertilizers as well as organic and other domestic fertilizers must be widely used in acid soils. The phosphorite treatment is the most economical procedure for increasing the phosphate level of the soil. Prospectively, application of phosphorite fertilizers in agriculture will be considerably expanded.

The main route to solve the grain problem is the introduction of intensive technology to raise the gross yield of grain to 255 million tons. This work has been well organized in the Krasnodar and Stavropol krays as well as in the Sumy and Khmel'nitskiy oblasts.

Considerable work is being accomplished by the agrochemical service in the organization of the complex application of chemical agents to agricultural crops, to be cultivated by industrial technology. In 1985, throughout the country, surplus yields of sunflowers, potatoes, sugar beets, corn and vegetables cultivated by industrial technology were obtained. However, we have still failed to realize all the possibilities of these technologies, especially in the non-chernozem zone of the RSFSR.

Special attention has to be paid to increasing yields by chemicalization on reclaimed soils. In many regions of the country, there are still serious deficiencies in this respect. The main causes of this situation are related to breakdown of technological discipline, obsolete methods of irrigation, shortage in fertilizers and other chemicals, high contamination of the crops, presence of large areas of acid and saline soils. On those fields, complex agrochemical treatment of young crops has to be assured and the latest advances in scientific technical progress need to be introduced.

Many farms of the Moldavian SSR have successfully applied technology in the irrigated territories. Optimization of the basic conditions in cultivation of corn (irrigation, balanced nutrients, the required thickness of plant arrangement) have secured a yield of 80-120 quintals of grain per hectare over extended areas in the 11th Five-Year Plan.

The use of fertilizers, herbicides, chemical meliorants with sprinkling cooling water is reducing labor expenditure by 25%, increasing the utilization factor of nutrients by 20-30% and productivity by 8-15%.

With intensive chemicalization of agriculture, the problems of environmental protection, especially of soil cover, water reservoirs and vegetable production become more serious.

Breaking rules in the application of nitrogenous fertilizers leads in many cases to an increased content of nitrates toxic for humans and animals in the vegetable products.

The agrochemical service must promote pollution control of agricultural objects by nitrates, pesticides, heavy metals and other toxic elements with special attention to selective control (checking, sampling) of nitrates in fruits and vegetable products, potatoes and green fodder. TsINAO, VIUA, the Department of Agrochemistry of TSKhA [Moscow "Order of Lenin" Agricultural Academy im. K. A. Timiryazev] have set regulations for the application of nitrogenous fertilizers for the main cultures. These regulations must be taken into consideration by the planning research institutes of chemicalization in devising the yearly plans for the fertilizers use on collective and state farms.

For practical acquisition of reliable information on soil productivity, quality of fodders and agricultural produces, fertilizers, chemical meliorants and for working out proposals and planning estimates for the complex application of chemical agents in agriculture, the Planning-Research Institutes of Chemicalization are well-equipped with new devices and machines. For example, automatic analytical systems and standardized devices are introduced, which permit improvement of the accuracy of the analytical work, increasing the labor productivity 2.5-3 times and expanding the collection of indices, including the determination of trace elements in soils and plants, and amino acids and vitamins in fodders.

In connection with the increase in the amount of fertilizers, chemical meliorants and pesticides used, the improvement of the material and technical basis of chemicalization, the equipping of Planning-Research Institutes of Chemicalization with modern and highly-efficient devices and machines, the role of the specialists of the agrochemical service, collective and state farms is assuring the highly effective application of chemical agents by using the latest advances of the scientific technical progress in agriculture.

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## CHEMISTRY OF CLUSTERS--ACHIEVEMENTS AND PERSPECTIVES

Moscow ZHURNAL VSESOUZNOGO KHIMICHESKOGO OBSHCHESTVA IM. D. I. MENDELEYEVA  
in Russian Vol 32, No 1, Jan-Feb 87 pp 3-11

[Article by S. P. Gubin, Institute of General and Inorganic Chemistry imeni  
N. S. Kurnakov, USSR Academy of Sciences]

[Abstract] The chemistry of clusters represents a new scientific direction combining work in a number of disciplines. This article reviews three types of metal-containing clusters: ultradispersed metallic clusters, cluster materials, and molecular cluster compounds of metals. The ultradispersed metallic clusters with diameter less than 300 Å often allow the formation of metastable structures and exhibit thermal, electromagnetic and other properties not typical of the bulk metal, alloy, or compound (such as nitride, boride, or carbide). Usually formed by some method of vapor condensation or explosive or chemical decomposition, uniform size dispersion remains a challenge, as does stabilization of the clusters once formed, a process often using ligands to reduce surface reactions of the cluster. Cluster materials are formed around metallic chains, rings, polyhedrons, or particles in a matrix of organic polymers or zeolites. These exhibit unusual properties and are a focal point of research on tailored conductors, including super-conductors. Cluster-containing zeolites also exhibit selective catalytic properties. Metallic clusters in organic polymers, termed "klaspol" materials, exhibit high thermal stability and unusual magnetic and electrophysical properties. Molecular cluster compounds contain a metallic skeleton in a framework of ligands, based on a kind of "organic" chemistry of noncarbon compounds. These are characterized by short (less than 3.5 Å) metal-metal bonds which can be classified by their convex polyhedral geometry and whose electron structure is much more complex than envisioned by classical coordination chemistry. Cluster chemistry has developed methods for generating polymetallic compounds with regular dispersion on an atomic level. Such polymetallic compounds can have complex stereosymmetry for use as specialized and highly active catalysts. These heterometallic clusters may be formed by direct substitution of one metal for another and can have strictly defined geometric and compositional structures, as illustrated by Fe-Rh systems. These can be decomposed into ultradispersed powders retaining the stereometric relationships of the metal skeletons. Notable recent achievements has been the synthesis of large and even gigantic (e.g., Pd<sub>561</sub>) clusters and an improved understanding of nucleation and particle growth in the formation of ultradispersed powders. Clusters



also act as biocatalysts and are present in many life forms, often in conjunction with specialized proteins, where they may also serve as transport mechanisms for specific metal atoms. Overall, cluster chemistry is a dynamic region of chemical development directly affecting a wide range of technical and technological areas. Figures 7; references 30: 17 Russian, 13 Western.

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## CHEMICAL BUILDING OF HETEROMETALLIC MAGNETICALLY ACTIVE CLUSTERS

Moscow ZHURNAL VSESOUZNOGO KHIMICHESKOGO OBSHCHESTVA IM. D. I. MENDELEYEVA  
in Russian Vol 32, No 1, Jan-Feb 87 pp 88-95

[Article by A. A. Pasynskiy and I. L. Yeremenko, doctors of chemical sciences,  
Institute of General and Inorganic Chemistry imeni N. S. Kurnakov, USSR  
Academy of Sciences]

[Abstract] Heterometallic clusters can be gradually built up by having metal complexes act as ligands with nonsaturated complexes of other metals. Complexes containing terminal or bridge donor atoms of nontransition elements of groups V and VI, particularly P and S, are widely used as such "building blocks." Magnetic clusters require high-spin complexes with metal-metal bonds. In particular, magnetically-active chalcocromite semiconductors have been obtained by reacting antiferromagnetic binuclear Cr complexes with various complexes of other transition metals. The antiferromagnetic cluster  $(C_5H_5)_2Cr_2(\mu-OCMe_3)_2$  reacts with Fe tetracarbonyl to form a heterometallic cluster having two Fe-Cr bonds of slightly different length (2.697 and 2.707 Å) without changing the length of the Cr-Cr bond (2.635 Å). An analogous cluster with tert-butyl mercaptyl ligands and a sulfide bridge replacing the Fe can be further complexed with  $(PPh_3)_2PdCl_2$  to form a cluster with the Cr-Cr distance of 4.078 Å, effectively breaking the Cr-Cr bond and greatly decreasing the antiferromagnetic interaction. Using Cr, Mo, or W carbonyls forms heterometallic complexes with the second metal linked to the S bridge and not the Cr. However, the reaction with Fe tetracarbonyl removes one of the tert-butyl groups and produces a complex with Fe-S bonds as well as two unequal Cr-Fe bonds (2.7 and 3.11 Å) due to an unpaired electron. Replacement of Fe with Mn produces a complex in which both Mn-Cr bonds are short (2.716 and 2.828 Å); similar clusters were also formed with Re and Co. The Co analog can then add an additional Co atom while removing the remaining tert-butyl group, forming a nearly symmetrical diamagnetic cluster with close Cr-S and Cr-Co bonds. An analogous cluster with pentadienyl nickel is less symmetrical and antiferromagnetic.  $(C_5H_5)_3Cr_3S_4CoCo$  has a symmetrical tetrahedral arrangement; the addition of two carbonyl groups to the Co greatly increases the Co-Cr distances. When reacted in pivalic acid, one S bridge is replaced by O, which hydrogen-bonds to a molecule of the acid. A similar cluster with Fe instead

of Co retains all the S bridges, but has a carboxyl group on the Fe. Cationic clusters with four Cr atoms also complex with Sn anions to form a paramagnetic cluster. Similar clusters with four V atoms in a tetrahedral arrangement are also paramagnetic. Antiferromagnetic clusters with a five-atom  $\text{Cr}_2\text{-Co-Cr}_2$  lattice were formed by the action of pivalic acid on the  $\text{Cr}_2\text{-Co}$  clusters obtained earlier. Replacing Co with Fe in a methylpentadienyl analog produced a cluster with unequal Fe-Cr bonds; a Mn analog of this cluster showed the steric effects of the methyl groups and the influence of a lower number of binding electrons in the metal lattice. Similar clusters with five Cr atoms and with substitutions of V and Ni were also formed. Overall, these syntheses show the potential of building tailored complexes on heterometallic lattices with tailored magnetic properties. References 35: 1 Russian, 34 Western (17 by the authors of this article).

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#### THIRD ALL-UNION SYMPOSIUM ON CHEMISTRY AND TECHNOLOGY OF HALCOGENS AND HALCOGENIDES

Alma-Ata VESTNIK AKADEMII NAUK KAZAKHSKOY SSR in Russian No 1, Jan 87 pp 78-90

[Article by B. Ye. Kozhakov, candidate of chemical sciences and B. K. Zhakibayev, candidate of technical sciences]

[Abstract] The symposium on the chemistry and technology of halcogens and halcogenides was held 24-26 September 1986 in Karaganda under the sponsorship of the Scientific Council for Inorganic Chemistry of the USSR Academy of Sciences, the Chemical and Metallurgical Institute of the Kazakh SSR Academy of Sciences, Karaganda State University and other related institutions in Kazakhstan. The reports (from numerous institutions in 19 cities of the USSR) were divided into sections on thermodynamics and kinetics of chemical processes using halcogens and ammonia; chemical properties of compounds based on halcogens; electrochemical transformations of substances containing halcogens in an aqueous medium; and technology and ecological considerations of processing materials containing halcogens. Physicochemical processes discussed included thermodynamics of evaporation, decomposition and transformations, computer processing of data related to halcogens and halcogenides; halcogenides of various metals and their properties and prospects; hydrometallurgical processing of copper sulfide concentrates and acid reduction of pyrrotines; the electrochemical behavior of halcogens and compounds containing them; halcogens in semiconductors; and technical and practical tasks required for the advancement of halcogen and halcogenide applications.

12131/5915  
CSO: 1841/271

CRYSTALLINE STRUCTURE OF  $[\text{NdCl}(\text{HMPA})_5](\text{PF}_6)_2$ 

Kiev UKRAINSKIY KHIMICHESKIY ZHURNAL in Russian Vol 53, No 3, Mar 87  
(manuscript received 20 May 86) pp 227-231

[Article by A. A. Kapshuk, V. M. Amirkhanov, V. V. Skopenko and  
V. S. Fundamenskiy, Kiev University]

[Abstract] Results are presented from an interpretation of the structure of the compound  $[\text{NdCl}(\text{HMPA})_5](\text{PF}_6)_2$ , obtained in the reaction, (in acetone solution),  $\text{NdCl}_3 \cdot n\text{H}_2\text{O} + 5\text{HMPA} + 2\text{NaPF}_6 \rightarrow [\text{NdCl}(\text{HMPA})_5](\text{PF}_6)_2 + 2\text{NaCl} + n\text{H}_2\text{O}$ .

Ethyl orthoformate was used as a dehydrating agent. The structure was interpreted by the heavy atom method. The coordinates of Nd were found from the three dimensional distribution of the Patterson function, that of the remaining 66 nonhydrogen atoms--from subsequent Fourier syntheses. The coordinates of all the atoms in the structure of the compound are presented in tabular form. X-ray structural analysis reveals that the HMPA molecules in the compound are in a sterically-hindered position, distorting the line and angle characteristics of the molecule of HMPA in comparison to known structural data. Figures 2; references 6: 5 Russian, 1 Western.

6508/5915  
CSO: 1841/292

CRYSTALLINE STRUCTURE OF BORIDE  $\text{Lu}_2\text{Ni}_3\text{B}_6$ 

Kiev DOKLADY AKADEMII NAUK UKRAINSKOY SSR: SERIYA B: GEOLOGICHESKIYE, KHIMICHESKIYE I BIOLOGICHESKIYE NAUKI in Russian No 2, Feb 87  
(manuscript received 15 May 86) pp 35-37

[Article by O. M. Dub, Yu. B. Kuzma, M. D. Mazus, N. F. Chaban and  
T. I. Malinovskiy, Lvov State University imeni I. Ya. Franko; Institute of  
Applied Physics, MSSR Academy of Sciences, Kishinev]

[Abstract] The authors report on discovery of the title compound while studying phase balance in an Lu-Ni-B system at 50-60% boron by atomic weight. Monocrystals were extracted from a two-phase specimen containing  $\text{LuB}_2$  and the boride studied; the sample had been obtained by melting Ni and B in lutetium in an argon medium. An automatic diffractometer was used to determine the structure, and atoms of the metals were identified by analysis of interatomic function and an electron density procedure. Computer processing using a program identified as XTLSM helped to delineate the structure as that of a coordinated multifaceted prism typical for ternary diborides. The coordination numbers of Lu, Ni and B atoms are 23, 12 and 9, respectively, and the structure is similar to that of  $\text{ThMoB}_4$ . Figures 2; references 4: 3 Russian, 1 German.

12131/5915  
CSO: 1841/265

ISOTHERMAL CROSS-SECTIONS OF STATE OF SYSTEM PRASEODYMIUM-NICKEL-GERMANIUM  
AT 870 (0 - 0.5 Pr) AND 670 K (AT 0.5 - 1 Pr)

Kiev DOKLADY AKADEMII NAUK UKRAINSKOY SSR: SERIYA B: GEOLOGICHESKIYE,  
KHIMICHESKIYE I BIOLOGICHESKIYE NAUKI in Russian No 2, Feb 87  
(manuscript received 27 Jun 86) pp 52-54

[Article by M. F. Fedina, V. K. Pecharskiy and O. I. Bodak, Lvov State  
University imeni I. Ya. Franko)

[Abstract] The authors report on study of the system Pr-Ni-Ge as part of a systematic study of germanium, iron and praseodymium. The present study focuses on examination of the crystalline structure using diffractometers and analyzing the data collected with a "PMNK" program on an SM-4 computer. Isothermal cross-sections of Pr-Ni-Ge systems show the solid binary states which formed; in all, seven new ternary compounds were studied, although the structure richest in praseodymium could not be analyzed due to the lack of monocrystals in the alloys produced. References 12: 8 Russian, 4 Western.

12131/5915

CSO: 1841/265

UDC 621.039.335

ONE-PHOTON ISOTOPICALLY SELECTIVE DISSOCIATION OF  $\text{CF}_2\text{Cl}_2$  MOLECULES IN FIELD OF RADIATION OF PULSED  $\text{CO}_2$  LASER

Moscow ZHURNAL FIZICHESKOY KHIMII in Russian Vol 61, No 2, Feb 87  
(manuscript received 3 Jun 85) pp 475-479

[Article by V. A. Kuzmenko]

[Abstract] A  $\text{CO}_2$  laser and the compound  $\text{CF}_2\text{Cl}_2$ , which has been previously examined, were used to study the conditions and mechanism of dissociation of molecules in the field of an IR laser. It was found that the thermal collision mechanism of dissociating activation of molecules predominated. The single-photon, isotopically-selective dissociation of molecules in the field of radiation in IR laser can be used to study the kinetics of chemical reactions under unstable conditions. By changing the delay between the laser pulse which heats the gas and the probing laser pulse, which performs single-photon isotopically selective dissociation, the kinetic of dissociation of molecules can be studied on the basis of the change in isotope composition of the dissociation products. Figures 4; references 13: 9 Russian, 4 Western.

6508/5915

CSO: 1841/302

UDC 541.123.2

STATE-DIAGRAM OF SYSTEM  $\text{BeO} \cdot \text{Al}_2\text{O}_3 - \text{Al}_2\text{O}_3$ 

Minsk DOKLADY AKADEMII NAUK BSSR in Russian Vol 30, No 10, Oct 86  
(manuscript received 3 Sep 85) pp 933-934

[Article by V. N. Matrosov, A. I. Alimpiyev and T. A. Matrosova, Experimental Production Enterprise for Manufacture of Unique Physical Instruments and Equipment, Scientific and Technical Association, USSR Academy of Sciences]

[Abstract] The system  $\text{BeO} \cdot \text{Al}_2\text{O}_3$  is interesting because it includes compounds which are promising for use in solid-state lasers. The authors studied the state-diagram of this system in the area from chrysoberyllium ( $\text{BeO} \cdot \text{Al}_2\text{O}_3$ ) to corundum ( $\text{Al}_2\text{O}_3$ ). In the process of studying the state-diagram of  $\text{BeO} \cdot \text{Al}_2\text{O}_3$  and growing chrysoberyllium (Alexandrite) crystals, the authors discovered the

existence of a low temperature modification of chrysoberyllium ( $\beta\text{-Be}\cdot\text{Al}_2\text{O}_3$ ) the structure of which was not established. This modification has a narrow area of existence near the melting point of chrysoberyllium. The compound  $\text{BeO}\cdot 3\text{Al}_2\text{O}_3$  was found to melt congruently at  $1867^\circ\text{C}$ . Figures 2; references 7: 5 Russian, 2 Western.

6508/5915  
CSO: 1841/304

UDC 621.372.8.666.22

# KINETICS OF FORMATION OF PLANAR WAVEGUIDES IN GLASSES BY ELECTRODIFFUSION OF SILVER

Leningrad FIZIKA I KHIMIYA STEKLA in Russian Vol 12, No 6, Nov-Dec 86  
(manuscript received 17 Apr 84; after revision 26 May 86) pp 676-681

[Article by I. A. Voytenkov and V. P. Redko]

[Abstract] The purpose of this work was to demonstrate the possibility of predicting the parameters of electrodiffusion waveguides as functions of manufacturing conditions. This is achieved by determining the basic characteristics of the electrodiffusion process and establishing the interrelationships among them and the parameters of the waveguides produced. The material used for the substrate was LK5 optical glass, containing (in mol. %) 82.0  $\text{SiO}_2$ , 11.0  $\text{B}_2\text{O}_3$ , 0.9  $\text{Al}_2\text{O}_3$ , 0.8  $\text{MgO}$  and 5.3  $\text{Na}_2\text{O}$ , plus technical glass for photographic plates containing 70.0  $\text{SiO}_2$ , 0.3  $\text{Al}_2\text{O}_3$ , 8.0  $\text{MgO}$ , 6.4  $\text{CaO}$  and 15.3  $\text{Na}_2\text{O}$ , with an oxidized silver film as a diffusant. The increment in the index of refraction caused by low temperature silver-sodium substitution in LK5 and technical glass was found to be constant at  $0.61 \pm 0.02 \text{ mol}^{-1}$ . The increment in index of refraction at the surface and its distribution through the depth of the waveguide layers formed by electrodiffusion of silver into these glasses can be predicted by means of the silver ion diffusion coefficient and sodium ion mobility, both of which are independent of concentration. Figures 4; references 13: 6 Russian, 7 Western.

6508/5915  
CSO: 1841/304

UDC 541.49:542.422:547.963.4

SYNTHESIS AND PHYSICAL-CHEMICAL PROPERTIES OF C-AMINOACYL DERIVATIVES OF PORPHYRINS AND METALLOPORPHYRINS

Ivanovo IZVESTIYA VYSSHIKH UCHEBNYKH ZAVEDENIY: KHIMIYA I KHIMICHESKAYA TEKHNLOGIYA in Russian Vol 30, No 1, Jan 87 (manuscript received 3 Jan 86) pp 3-16

[Article by V. N. Luzgina, Ye. I. Filippovich and R. P. Yevstigneyeva, Department of Chemistry and Technology of Fine Organic Compounds, Moscow Institute of Precision Chemical Technology imeni M. V. Lomonosov]

[Abstract] Hemoproteins, differing in structure and functions, always contain an iron-porphyrin complex in the active center of the macromolecule, complexly bonded with the protein. This article studies means and methods of synthesis of C-aminoacyl derivatives of porphyrins and metalloporphyrins, particularly C-aminoacyl peptide derivatives of protohemin IX. The catalytic activity of these derivatives is described, as well as their use in the study of the properties of key enzymes in prostaglandin synthesis. Chlorophyll-protein interactions are modeled using C-aminoacyl derivatives of protohemin IX. Figures 4, references 58: 20 Russian, 38 Western.

6508/5915  
CSO: 1841/296

UDC 547.979.733

SYNTHESIS AND PROPERTIES OF PORPHYRINS IN THE PROTOPORPHYRIN IX GROUP

Ivanovo IZVESTIYA VYSSHIKH UCHEBNYKH ZAVEDENIY: KHIMIYA I KHIMICHESKAYA TEKHNLOGIYA in Russian Vol 30, No 1, Jan 87 (manuscript received 5 Jul 85) pp 48-51

[Article by A. S. Semeykin, M. B. Berezin, O. I. Koyfman and G. A. Krestov, Department of Chemical Technology of Plastics and Film Materials, Ivanovo Institute of Chemical Technology; Institute of Chemistry of Nonaqueous Solutions, USSR Academy of Sciences]

[Abstract] Protoporphyrin IX, the main structural unit of hemoglobin, cytochromes and several enzymes, has attracted the attention of scientists. This article suggests a method for demetallizing and esterification of hemins.

Esterification was performed in methanol by a solution of HCl obtained by interacting methanol with acetyl chloride, eliminating the need to dry the reagents. The method allows rapid production of porphyrins in large quantities. PMR spectra were recorded. References 6: 1 Russian, 5 Western.

6508/5915  
CSO: 1841/296

UDC 547.1'13+541.127

#### HETEROGENEOUS DECOMPOSITION OF CHROMIUM BISARENES ON METALLIZED SURFACE

Leningrad ZHURNAL OBSHCHEY KHIMII in Russian Vol 57, No 2, Feb 87  
(manuscript received 10 Feb 86) pp 364-368

[Article by L. M. Dyagileva, Ye. I. Tsyganova and Yu. A. Aleksandrov, Scientific Research Institute of Chemistry, Gorkiy State University imeni N. I. Lobachevskiy]

[Abstract] A study is reported of the kinetics of heterogeneous pyrolysis of chromium ethylbenzene-diethylbenzene on quartz metallized with pyrolytic chromium. Thermolysis was performed in an open system in a stream of helium at near atmospheric pressures by gas chromatography at 440-520°C, initial concentration  $1.5-3.5 \cdot 10^{-5}$  mol/l in the kinetic mode in an area with no external or internal diffusion limitations. The experiments showed that the products of decomposition of the initial compound--benzene, ethylbenzene--are weakly adsorbed by the pyrolytic chromium and do not poison the surface but rather are extracted from it by the chromium ethylbenzene and diethylbenzene. The kinetic and adsorption data suggest a mechanism for the decomposition reaction in which the limiting stage is decomposition of the adsorption chromium bizarene complex. References 7: 6 Russian, 1 Western.

6508/5915  
CSO: 1841/301

UDC 547.246

#### SYNTHESIS OF CARBOFUNCTIONAL ORGANOGERMANES CONTAINING ADAMANTYL AMINE AND ADAMANTYL AMIDE GROUPS

Leningrad ZHURNAL OBSHCHEY KHIMII in Russian Vol 57, No 2, Feb 87  
(manuscript received 17 Feb 86) pp 387-391

[Article by T. K. Gar, O. N. Chernysheva, A. V. Kisin and V. F. Mironov, State Scientific Research Institute of Chemistry and Technology of Heteroorganic Compounds, Moscow]

[Abstract] It is known that 1-aminoadamantane and 1-alkylaminoadamantane have neutrotropic and antiviral activity. During a search for biologically active compounds of germanium, the authors synthesized a number of derivatives



containing the  $1\text{-AdNHC(O)-R-Ge}\equiv$  and  $1\text{-AdC(O)N-R-Ge}\equiv$  groups, where R is an alkylene. This compound or its trimethylsilyl derivative were reacted with acid chlorides and esters. The N-chloromethyl derivative of 1-adamantane carboxylic acid amide is condensed with trichlorogermanium etherate to form 1-adamantane carboxylic acid N-trichlorogermymethyl amide. The possibility is shown of converting germyl-containing amides to the corresponding 1-amino-adamantane derivatives by reducing the amides with lithium aluminum hydride. References 5: 4 Russian, 1 Western.

6508/5915  
CSO: 1841/301

UDC 546.841.4.791.4

#### URANIUM (IV) AND THORIUM HALOGEN ACETATES

Moscow DOKLADY AKADEMII NAUK SSSR in Russian Vol 292, No 5, Feb 87  
(manuscript received 15 Apr 86) pp 1148-1153

[Article by Academician V. I. Spitsyn, K. M. Dunayeva and Yu. S. Matveyev,  
Moscow State University imeni M. V. Lomonosov]

[Abstract] Methods were developed or improved for synthesis and isolation in solid form of compounds of uranium (IV) and thorium with halogen-substituted acetic acid. The properties of the compounds produced were studied. Significant attention is given to processes of thermolysis of halogen acetates, since this may result in the formation of uranium (IV) and thorium halides which are promising for nuclear power engineering. All the compounds synthesized were solid crystalline substances. The IR spectra indicate that upon transition from tetraacetates to halogen acetates, the polymer structure of the uranium (IV) and thorium tetraacetates breaks down and is transformed to an ionic structure. The intermediate products of decomposition of the carboxylates are oxocompounds or carboxylate halides. Thermolysis of monoiodoacetates is accompanied by intermediate formation of carbonates, and the end products of decomposition are as follows: For monohalogen acetates--metal dioxides, for the other halogen acetates--tetrahalides or their mixtures with oxohalides. The decomposition process is explained as the formation of dioxides upon pyrolysis of the monohalogen acetates and the appearance of halides of various compositions upon pyrolysis of di- and trihalogen acetates, plus free carbon. Figure 1; references 5: 3 Russian, 2 Western.

6508/5915  
CSO: 1841/297

## THERMOCHEMISTRY OF 1, 1'-DI-N-BUTYLURANOCENE

Leningrad RADIOKHIMIYA in Russian Vol 29, No 1, Jan-Feb 87  
(manuscript received 28 Feb 86) pp 109-111

[Article by N. T. Kuznetsov, V. A. Mitin, K. V. Kiryanov, V. G. Sevastyanov  
and V. A. Bogdanov]

[Abstract] The enthalpy of combustion, temperature dependence of saturated vapor pressure and thermal behavior of 1, 1-di-n-butyluranocene uranium are studied by differential thermal analysis and high temperature spectrophotometry. The melting point and beginning of thermal decomposition, enthalpy of melting and evaporation, standard enthalpy of formation in condensed and gaseous states and mean energy of dissociation of the uranium n-butyluranocene bond are calculated. As in previous works, only a slight change in position and width of ionization bands is observed in comparison with unsubstituted uranocene, independent of donor-acceptor properties of the substituent. This is apparently explained by the capability of the central uranium atom to compensate for changes in electron density created by the ligands. References 12: 10 Russian, 2 Western.

6508/5915  
CSO: 1841/300

INFLUENCE OF NATURE OF PHASE EQUILIBRIUM ON CRYSTALLIZATION KINETICS OF  
 $\text{Ga}_{1-x}\text{In}_x\text{P}_{1-y}\text{As}_y$  SOLID SOLUTIONS

Moscow ZHURNAL FIZICHESKOY KHIMII in Russian Vol 61, No 2, Feb 87  
(manuscript received 19 Jun 85) pp 398-403

[Article by P. P. Moskvina and V. S. Sorokin, Leningrad Institute of Electrical Engineering imeni V. I. Ulyanov (Lenin)]

[Abstract] The process of crystallization of  $\text{Ga}_{1-x}\text{In}_x\text{P}_{1-y}\text{As}_y$  has been studied in a series of previous works, which have used a model of diffusion-limited crystallization to find the variation in properties of  $\text{Ga}_{1-x}\text{In}_x\text{P}_{1-y}\text{As}_y$ -InP heterostructures as a function of the parameters of the technological cycle. This article in the series analyzes the influence of crystallization conditions on the parameters of layers of the solid solution, comparing experimental and calculated results with analogous data obtained in the approximation of diffusion-limited growth. The results indicate that the nature of phase equilibrium is of major importance in liquid-phase epitaxy of multicomponent solid solutions. The model of complete mixing can be successfully used to select conditions for precipitating a solid solution. Figures 5; references 11: 5 Russian, 6 Western.

6508/5915  
CSO: 1841/302

DISSOCIATION ENTHALPY OF GAS PHASE COMPLEX MOLECULES IN SYSTEMS NaI-DyI<sub>3</sub> AND CsI-HoI<sub>3</sub>

Moscow ZHURNAL FIZICHESKOY KHIMII in Russian Vol 61, No 2, Feb 87  
(manuscript received 22 Jan 86) pp 512-514

[Article by Ye. N. Gavrilin, N. S. Chilingarov, Ye. V. Skokan, I. V. Scrokin, O. Kaposhi and L. N. Sidorov, Moscow State University, imeni N. V. Lomonosov, Department of Chemistry]

[Abstract] This work concerns determination of the enthalpy of dissociation of the complex molecules NaDyI<sub>4</sub>, Na<sub>2</sub>DyI<sub>5</sub> and CsHoI<sub>4</sub>, Cs<sub>2</sub>HoI<sub>5</sub> in the gas phase. Studies were performed on a modified MI-1201 mass spectrometer with ionizing electron energy 50-70 eV. A nickel effusion Knudsen cell was used as the source of the molecular beam, formed by evaporation of the initial experimental charges, containing 80 mol.% of the iodides of dysprosium and holmium. References 8: 4 Russian, 4 Western.

6508/5915  
CSO: 1841/302

UDC (546.821/824+546.74+547.58)541.49

## COMPLEX COMPOUNDS OF TITANIUM (IV) AND NICKEL (II) WITH AROMATIC ACIDS AND THEIR DERIVATIVES

Tashkent UZBEKSKIY KHIMICHESKIY ZHURNAL in Russian No 6, Nov-Dec 86  
(manuscript received 6 Dec 85) pp 7-10

[Article by Z. Sh. Fayzutdinova, K. S. Khakimova and Ya. Medvedskaya, Tashkent Pharmaceutical Institute]

[Abstract] Synthesis of coordinated compounds of trace elements with bioactive ligands to produce biostimulants and other medications has become an important field of bioinorganic chemistry. The present article reports on coordination of titanium and nickel with salicylic acid, para-aminosalicylic acid and salicylic acid amide. After crystals were formed and dried, their infrared spectra were studied. Compounds analyzed were Na<sub>2</sub>[Ti(SA")<sub>3</sub>]·5H<sub>2</sub>O, Na<sub>2</sub>[Ti(PASA")<sub>3</sub>]·6H<sub>2</sub>O, Ni(PASA')<sub>2</sub>·4H<sub>2</sub>O, NiCl<sub>2</sub>PASA, Ni(ASA)<sub>2</sub>·H<sub>2</sub>O. Study of infrared spectra of phenol-hydroxyl, carboxylation, free phenols and the metals indicated that among other reactions the hydrogen of the carboxyl group was replaced by the metals, with the hydrogen ion migrating to the amino-group and forming an N<sup>+</sup>H<sub>3</sub> group, to which a chlorine ion attaches by an ion bond. Structural diagrams are presented for the key complexes. References 4: 2 Russian, 2 Western.

12131/5915  
CSO: 1841/284

DELAY IN NEW COKING TECHNOLOGY USING SUBSTANDARD COAL

Kiev RABOCHAYA GAZETA in Russian 24 Mar 87 p 2

[Article by Yu. Kovalenko, special correspondent for RABOCHAYA GAZETA, Dnepropetrovsk--Dneprodzerzhinsk--Kharkov: "For the 31st Year; Why Technology Capable of Marking a New Day in the By-Product Coke Industry Risks Finding Itself Taking a Back Seat in Scientific and Technical Progress"; first paragraph is source introduction]

[Text] The Work Force of Science

Thirty years ago Moscow scientist L.M. Sapozhnikov proposed a basically new method of coking, thanks to which it was possible to produce blast-furnace raw material not only from coking coals but also from ordinary ones, practically from coal dust. The new technology guaranteed a sharp improvement in the ecological situation at coke chemical enterprises. In addition, it freed people of heavy, harmful labor.

Yu.B. Tyutyunnikov returned elated from Novokuznetsk. A decision was signed on the construction of an installation for form coke. They had taken the trip to resolve the design. The initiative for which they had struggled for many long years had won out.

Adopting L.M. Sapozhnikov's idea, specialists of the Kharkov Coal Chemistry Institute, with the active participation of staff members of the Eastern Coal Chemistry Institute and planners, advanced the idea to planned development. Practically any coal gas, weakly sintering, as they say, long-flame fuel can be caked, producing an excellent blast-furnace raw material.

Back in the '60s, a small installation was established in Kharkov. Coal usually burned in ovens is changed into coke in them. But it was necessary to verify the technical solutions on an industrial scale, to get official approval for the actual organization of the process and to bring to a logical conclusion the design findings. And shortly right there in Kharkov, an installation began operating with the projected capacity of 10,000 tons of form coke a year. This was already in the middle of the '70s.

The UFK [expansion unknown] as its creators called it, confirmed the validity of the scientific preconditions and the importance of the technical solutions.

Now it was only necessary to prove the economic feasibility and the economic effectiveness of the new coking method. This is how the idea was born to build the first installation in Novokuznetsk with a capacity of 500,000 tons of coke a year. This was not simply a success crowning a long scientific search. A truly full measure of human patience was required to defend the idea and to prove its competence. How could one not rejoice here?

Alas, the joy of Tyutyunnikov and his colleagues was premature. In Novokuznetsk, the construction project folded without being able to develop momentum. Even the reasons for such a rash decision by the Kharkov specialists remain unknown. However, it was planned to build two sections for the production of form coke in Altay. But again a setback....

The years passed. And at last, finally, a decision was adopted to build a corresponding installation at the Dnepropetrovsk By-Product Coke Plant imeni Kalinin. This time it was not the scientists but the production people, particularly the enterprise director himself, A.G. Nechayev who fought for the form coke.

Anatoliy Georgiyevich had a real personal interest in it. The question of modernization was put squarely before the plant. They wanted to carry it out on a new technical level. It would be necessary to create favorable conditions for the workers and for the environment. After all, the plant was located in an area where ecological problems were quite substantial, while present technologies do not ensure cleanliness of the air environment [vozdushnyy basseyn]. The fact is that in the production of form coke, harmful emissions are reduced to a minimum. The worker is transformed into an operator in elegant coveralls. There are no smoke trails harmfully affecting the health of people. It is necessary to also take into account raw-material problems--there is less and less coking coal.

Nechayev went as far as Moscow fighting for renewal of the plant on a new technical basis. It seemed as if everything was decided. Before long modernization of the enterprise got underway and batteries were overhauled according...to traditional technology--dirty, smoky, unattractive. The plan for the new installation was placed under wraps.

"The only objection to form coke," B.I. Meniovich, chief of an integrated department of Giprokoks [expansion not available], says with regret, "is that it is more expensive than that produced in the traditional way." Although this is debatable. After all, the special features of the new method have not been taken into account. In the case of traditional technology, millions of rubles are required for the construction of nature conserving structures. Furthermore, with the old technology, it was only possible to obtain high-quality coke with some types of coal which are more expensive and whose reserves, as we know, are being reduced. But the new installation, as has already been said, can work with any coal. Consequently, the design for the Dnepropetrovsk plan eventually was adopted, having passed Glavekspertiz [expansion not available]. It was also approved by Gosplan and Gosstroy. And then unexpectedly doubts appeared at the concluding stage....

Still, hopes were not decisively shattered. Another decision appeared--to build the UFK at the Bagleyskiy By-Product Coke Plant in Dneprodzerzhinsk. True, here the estimated price for the future form coke had grown 1.5-fold--it was necessary to provide additional protection against emissions. A complex was planned basically for the gas and weakly sintering coal of the Western Donbas. It is close by and the delivery costs are minimal. Yet its price soared for some reason and became the same as for first-grade coking or soft coal. So the anticipated economic effect was reduced.

In a word, the construction of the installation at the Bagleyskiy plant, although it has started, it is proceeding, as they say, fair to middling. In four years, 7 million rubles failed to be used. Last year, hardly half of the planned work was completed.

Meetings of the scientific council "New Processes in the By-Product Coke Industry" of the USSR State Committee for Science and Technology were held twice at the enterprise. But even this was unable to spur on progress of the work.

"The main thing that is bothersome in this matter," pointed out V.A. Kuzmin, the plant's director, "is that such units took too long to pay back for themselves. But at the same time, other advantages have not been taken into consideration. If the UkSSR Ministry of Ferrous Metallurgy were to elucidate them clearly, form coke would by now have been long available."

The ministry's policy really is not distinguished for its consistency. First, they grabbed hold of a technology of partial briquetting purchased from Japan. The money was considerable. And the prokuto [?]? This method requires a binder, which is not produced in the country. The petroleum people seemingly are promising to create it. Many specialists are uncertain but assert that in Kommunarsk an installation should be created for the production of coke from compacted charge. Also a foreign technology. But actually this does not solve anything from the point of view of improving the ecological situation. And for Dneprodzerzhinsk this problem is particularly acute. The Bagleyskiy plant receives a great many instructions from nature-conservation organizations.

"It is necessary to do something," V.A. Kuzmin says. "It cannot continue in this way indefinitely," and points to the clouds of smoke rising outside the window.

The advantage of form coke lies not only in the possibility of using substandard coal. It is perhaps no less important that this is entirely a domestic technology that excludes bringing in extra equipment.

With respect to a method that is domestic and one's own, as shown by the facts, the attitude is clearly disdainful. Of more than 300 million rubles allocated for the development of new coking technologies, the lion's share has been allotted for partial briquetting and ramming. And only 18.2 percent for form coke. These data were obtained at the Kharkov Engineering Economics Institute, in the department where the same Yu.B. Tyutyunnikov works.

And these are not just figures. This is the position of the UkSSR Ministry of Ferrous Metallurgy. And it is mirrored at the construction site.

While visiting there we ran into R.S. Baranov, the brigade leader of Avdeyevskoye Construction Administration No 227 of Koksokhimteplomontazh Trust.

"Two of our brigades work here--15 persons," he said. "The administration's chief V.I. Mikitan recently phoned. He said that if there is a work front he could send another brigade to create a second shift. But so far we have been able to handle the volume. There are also people working from the komsomol Kharkovstalkonstruktsiya Sector. And that is all."

"But in order to create an adequate work front for all the participants, 400-500 people would be required," installation chief Ye.S. Matveyev morosely commented. "We don't even have half. Hence the results."

Incidentally, all the mixups in the construction of the installation for form coke could have been foreseen in good time. And the ones to blame for them are none other than the UkSSR Ministry of Ferrous Metallurgy and Ukrkoks [expansion not available] in particular. The fact is that it was planned to start the modernization of the Bagleyskiy plant after the installation became operational. It would have taken on a part of the production volume. But the work on the UFK barely got started when they began to rebuild the existing batteries. And as the builders assert, they "snatched" for this a part of the money allocated for the new installation. And so the construction project has become a secondary if not a tertiary item.

All this expenditure of construction efforts was known in advance by the republic's Ministry of Ferrous Metallurgy. We can say that the general contractor, the Dzerzhinskstroy Trust, is so overloaded that even while fulfilling annual plans 140-150 percent, it cannot improve all the facilities--the oxygen converter shop, the rolling mill and rebuilding of the ovens for Dneprodzerzhinsk and the same Bagleyskiy by-product coke plants. What can you expect?

In 1985, as had been planned, the installation had not been turned over. In 1988, as designated by the corrected plan, coke will hardly be produced. A case of classical "dolgostroy" ["long-time construction"]!

An almost theatrical act was played out recently at an operations conference held at the Bagleyskiy plant. Scientists of the Scientific-Research Institute of Coal Chemistry who were recently criticized at a plenum of Kharkov Gorkom for their slowness raised the question: when will the installation start up?

A representative of the general contractor, who led the operations conference, replied without batting an eye:

"As specified in the plan--in 1988."

"If they order it, we would turn it over," N.A. Zhidko, deputy chief of the Dneprometallurgstroy Combine, clarified the categorical position of the

chairman. "We shall turn it over without fail!" But at the same time he added on his own: "If they so order it."

But it is high time that it be so ordered. Because the new technology risks taking a back seat in scientific and technical progress. The fact is that not a single word was mentioned in the report on the discussions and assurances at the operations conference. The startup of the progressive installation capable of marking a new day in by-product coke chemistry is quite problematic.

7697

CS0: 1841/291



RESOURCEFUL INCREASE OF PETROLEUM RECOVERY IN FALLING YIELD AREA

Moscow SOTSIALISTICHESKAYA INDUSTRIYA in Russian 24 Apr 87 p 1

[Article by A. Cherkasov, general director of the Permneft Association, Perm: "Together with Partners"; first paragraph is source introduction]

[Text] The collective of the Permneft Association in the first quarter provided the country 15,000 tons of additional production. The confident start prompted the oil-field workers to revise their initial commitments. They gave their word to raise the above-plan count to 15,000 tons of oil by the end of the year.

In the Kama area, there are no Tyumen Samotlorovs. More than a half century has passed since industrial development of the deposits first started. Big deposits have largely been exhausted. The Kama area has become a region with a falling yield. The decline was explained by objective circumstances. But in their heart, they did not feel right: the professional pride of the oilworkers gave them no peace. Is it really not possible to increase the yield of the beds?

Here is the story of the Severokamskoye deposit. Adherents of traditions got ready to shut down because of the low profitability of the production shop here. A creative group decisively opposed this. It was formed and headed by V. Viktorin, chief of the development department.

They took a chance. For two years, they shut down all producing wells and started to use them as injection wells. Water was injected deep under. It not only increases pressure in the beds but also washes out the petroleum which lies hidden in nooks and crannies. Then production was renewed. And the underground storeroom began to surrender its contents.

The method turned out to be highly effective. The volume of extracted petroleum increased tenfold, while its production cost was reduced sixfold. The shop at the Severokamskoye deposit is now operating with a normal load.

In February of last year, the association's collective adopted the developed program of stabilizing output. We determined the limit--to produce 11,400,000 tons yearly. This is a limit below which we do not have the right to go. In

the course of the five-year plan, we shall give the country 1,200,000 tons of hydrocarbon raw material above the control target.

The methods of maintaining formational pressure by pumping in water are well known. They are widely used in the Kama area.

Here we are helped out by a contract on cooperation with subcontractors with the slogan "From oil well to consumer." For example, the Permnefteorgsintez Association has committed itself to now produce an additional 20,000 tons of gasoline and many other kinds of fuel. We, in turn, have to send them 80,000 tons of above-plan petroleum. Common commitments, common concerns. The oil refiners supply us with their production wastes that serve as good solvents needed for intensification of petroleum recovery.

We are improving work contacts with other enterprises in the oblast. We know that together with petroleum a large amount of bed water comes up. Then it is repumped deep under for maintenance of pressure. And everything would be fine if the water did not possess great corrosive action. Each year it is necessary to replace more than 100 kilometers of water pipe.

We reached an accord with the Berezniki Azot Association to set up production of an inhibitor from the wastes--a substance increasing metal resistance. We helped organize this work and provided the subcontractors with the necessary equipment. As a result, Azot enjoys an extra profit, and the petroleum workers are the gainers.

We are improving cooperation with neighbors from other departments, yet with our own ministry we sometimes cannot find a common language. For example, we started experimental industrial pumping of the alkali instead of water into the bed. The gain is self-evident: in the Gozhanskaya area alone, it made it possible to extract 40,000 tons of petroleum more than heretofore. But, alas, the innovation has not found wide-scale employment. This year, we were allocated ministry funds for 1,600 tons of alkali below the planned amount.

We also ran into obstacles in another strategic direction--accelerated development of new underground storage areas. Here the main principle is: "Petroleum--on the cutting edge of a chisel?" Our shaft sinkers literally are straining ahead--they drilled more than 150 wells as opposed to 130 under the plan. We are especially happy with the achievements of brigade foreman N. Moiseyev from Berezniki, which were double the average sinking for the association.

We are happy for a special reason: the development of Bereznikovsko-Krasnovisherskiy Rayon is one of the decisive factors in the stabilization program. Here for the first time in world practice our specialists ran into the problem of working petroleum deposits on the territory of a potassium deposit.

The work, which continued for more than 10 years, confirmed the reliability of the found solutions. Two years ago, the union ministries of geology and the petroleum industry and Gosgortekhnadzor [State Mining Technical Surveillance] adopted a decision on the accelerated development of petroleum resources in

the north of the Kama area. However, its realization was constantly hindered in coordination of concrete plans, first of all with the management of the Perm Okrug of Gosgortekhnadzor SSSR [USSR State Mining Technical Surveillance] and the Uralkaliy Association. In brief, here you have had so far spinning wheels instead of acceleration.

Recently, a TASS report was published in the press about two underground nuclear explosions in Perm Oblast. They were carried out on the request of oilworkers. The purpose was to increase the recovery of liquid fuel from tiny lentil-shaped deposits. We are counting on significantly boosting the coefficient of petroleum recovery with the help of the peaceful atom.

7697

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UDC 577.391:615.42

STABILITY OF TERRYLITIN, CHEMICALLY BONDED WITH POLYMER, AGAINST EFFECTS  
OF  $\gamma$ -RADIATION

Ivanovo IZVESTIYA VYSSHIKH UCHEBNYKH ZAVEDENIY: KHIMIYA I KHIMICHESKAYA  
TEKHOLOGIYA in Russian Vol 30, No 1, Jan 87 (manuscript received 24 Jun 85)  
pp 117-118

[Article by T. N. Yudanov, I. F. Skokova, Ye. V. Dovbiy and A. T. Kalashnik,  
Department of Chemical Fiber Technology, Moscow Textile Institute imeni A. N.  
Kosygin; "Khimvolokno" Scientific-Production Association]

[Abstract] The authors have developed continuous methods for immobilization of proteolytic enzymes such as terrylitin on modified and unmodified cellulose materials. Gamma radiation is used to sterilize the materials. During irradiation, the free valence of terrylitin is transferred to the macromolecules of the polymer carrier. If this process is accompanied by recombination of macroradicals, the number of free radicals on the polymers containing the immobilized terrylitin will be less than on the polymer carriers. When terrylitin is  $\gamma$ -irradiated without a polymer carrier which is a radical acceptor, its proteolytic activity is greatly decreased by the formation of intramolecular and intermolecular bonds, changing the conformation of the enzyme macromolecule or damaging its active center. EPR data thus indicate that in materials containing immobilized terrylitin,  $\gamma$ -radiation causes migration of the terrylitin free valence to the macromolecules of the polymer carrier, as well as recombination of terrylitin radicals with the radicals of the cellulose carriers, stabilizing the enzyme against further  $\gamma$ -radiation. References: 4 Russian.

6508/5915  
CSO: 1841/296

# X-RAY FLUORESCENCE MONITORING OF CONTENT OF GADOLINIUM IN PLASTIC SCINTILLATORS BASED ON POLYMETHYL METHACRYLATE

Moscow ZHURNAL ANALITICHESKOY KHIMII in Russian Vol 42, No 2, Feb 87  
(manuscript received 18 Nov 85) pp 358-360

[Article by A. B. Blank, V. G. Vlasov, Z. M. Nartova and N. I. Shevtsov, All-Union Scientific Research Institute of Single Crystals, Scintillation Materials and Highly Pure Chemical Substances, Kharkov]

[Abstract] The purpose of this work was to prepare synthetic specimens of polymethyl methacrylate with known gadolinium content and use them for x-ray fluorescence determination of gadolinium in polymethyl-methacrylate-based plastic scintillators. With identical treatment of the analyzed and standard specimens, the systematic error of the analysis results is slight. Polished-surface radiators are preferable for analysis. The limit of detection is  $2 \cdot 10^{-4}\%$ . Figure 1; references 7: 4 Russian, 3 Western.

6508/5915  
CSO: 1841/306

# STRUCTURE AND CHARACTERISTICS OF HYDROGELS FORMED BY POLYACRYLIC ACID-POLYETHYLENEIMINE COMPLEXES

Moscow VYSOKOMOLEKULYARNYYE SOYEDINENIYA in Russian Vol 29, No 3, Mar 87  
(manuscript received 27 Jul 85) pp 517-524

[Article by Ye. M. Kopylova, S. P. Valuyeva, B. S. Eltsefon, V. B. Rogacheva and A. B. Zezin, All-Union Scientific Research Institute of Medical Polymers]

[Abstract] A combination of IR spectroscopy and potentiometric analysis was employed in structural studies on cross-linked hydrogels formed by polyacrylic acid-polyethyleneimine complexes. The complexes were determined to consist of a three-dimensional network of polymeric chains joined by ionic bonds. The number of such bonds may vary from ca. 65% in neutral media to virtually complete absence in strongly acidic or alkaline solutions, as well as in high concentrations of low-MW salts. At pH>8 the hydrogels undergo dispersion, with complete solubilization at pH>9. In acidic conditions, the gel structure persists despite the loss of ionic bonds due to the formation of hydrogen bonds between the carboxyl groups. The properties of the complexes in question were thus demonstrated to be amenable to modification by altering the number of stabilizing ionic, covalent and hydrogen bonds. Figures 4; references 10: 9 Russian, 1 Western.

12172/5915  
CSO: 1841/288

## FLOW CHARACTERISTICS OF POLYPROPYLENE-POLYSTYRENE MIXTURES WITH COAXIAL PHASE STRUCTURE

Moscow VYSOKOMOLEKULYARNYYE SOYEDINENIYA in Russian Vol 29, No 3, Mar 87  
(manuscript received 1 Aug 85) pp 579-582

[Article by Yu. P. Miroshnikov and Ye. N. Andreyeva, Moscow Institute of Fine Chemical Technology imeni M. V. Lomonosov]

[Abstract] A study was conducted on the flow characteristics of a mixture of polypropylene-polystyrene mixtures in which a coaxial (telescopic) phase structure was formed during capillary extrusion in a viscometer. The polymers were layered, one polymer above the other, to form a series of disks in the holding chamber. Reducing the thickness of the disks from 0.8 to 0.2 mm resulted in a 2- to 4-fold decrease in the viscosity of the mixture with the coaxial structure. Under appropriate conditions of disk thickness and pressure, a 17-fold reduction in viscosity was possible, attributable to interphasic slippage. Figures 3; references 5: 3 Russian, 2 Western.

12172/5915  
CSO: 1841/288

## INTERACTION OF PROTEIN MOLECULES WITH LINEAR POLYELECTROLYTE IN SOLUTION

Moscow VYSOKOMOLEKULYARNYYE SOYEDINENIYA in Russian Vol 29, No 3, Mar 87  
(manuscript received 5 Aug 85) pp 593-597

[Article by Ye. V. Anufriyeva, V. D. Pautov, N. P. Kuznetsova, V. B. Lushchik and M. G. Krakovyak, Institute of High Molecular Weight Compounds, USSR Academy of Sciences]

[Abstract] Luminescent polarization was employed in measuring the relaxation times of lysozyme:polymethacrylic acid (PMA) complexes, in order to assess the stability of the interaction over a wide range of lysozyme:PMA ratios ( $n$ ). In salt solutions, maximum stability was obtained at  $n = 1$ . At  $n = 1$  the percentage of free or unoccupied PMA sites was equal to 66%, while at  $n = 3$  virtually all of the PMA binding sites were occupied. Above  $n = 3$  a considerable portion of the lysozyme molecules were not incorporated into the compact protein:PMA structure, but adhered to the surface of the macromolecular complexes. In the latter case, particularly at  $n = 5$ , the complexes showed considerable loss of stability. Figures 6; references 8: 5 Russian, 3 Western.

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CSO: 1841/288

UDC 538.799.5

REDUCTION OF URANIUM (VI) TO URANIUM (IV) BY HYDRAZINE IN EMULSION OF  
AQUEOUS SOLUTION OF NITRIC ACID PLUS 30 VOL-PERCENT SOLUTION OF  
TRI-N-BUTYLPHOSPHATE (TBP)

Leningrad RADIOKHIMIYA in Russian Vol 29, No 1, Jan-Feb 87  
(manuscript received 8 Jul 85; in final form 18 Jul 86) pp 17-21

[Article by A. S. Solovkin and V. I. Druzherukov]

[Abstract] Tetravalent uranium stabilized with hydrazine is used in regeneration of spent nuclear fuel to reduce plutonium (IV) to plutonium (III). The authors have found that, at high temperatures in aqueous nitric acid solutions, hydrazine reduces  $U^{(VI)}$  to  $U^{(IV)}$ , the process occurring at a significant rate only at temperatures over  $60^{\circ}C$ . The reduction reaction has an induction period which depends on temperature and concentration of  $HNO_3$  and  $N_2H_4$ . The process reaches equilibrium in not over 5-6 hours as a result of oxidation of  $U^{(IV)}$  to  $U^{(VI)}$  by nitric acid. In a boiling water bath, the system does not reach equilibrium, and the concentration of  $U^{(IV)}$  in the aqueous and organic phases passes through a clear maximum. The reduction process is a zero-order reaction with respect to uranium, a first-order reactions with respect to hydrazine. The order of the reaction with respect to  $HNO_3$  is 3.5. The activation energy is 105kJ/mol. Figures 2; references 11: 8 Russian, 3 Western.

6508/5915  
CSO: 1841/300

UDC 535.376:546.799.6:564.65

RADIOLUMINESCENCE OF CURIUM (III) AND LANTHANIDES IN AQUEOUS SOLUTIONS

Leningrad RADIOKHIMIYA in Russian Vol 29, No 1, Jan-Feb 87  
(manuscript received 24 Feb 86) pp 118-121

[Article by A. B. Yusov]

[Abstract] The purpose of this work was to measure the yields of radioluminescence of curium and the lanthanides Tb, Eu, Dy and Sm under identical conditions, relating the values obtained with the quantum yields of photoluminescence of these ions and explaining the regularities observed. Radioluminescence yields were calculated by comparing them with the radioluminescence

yield of curium obtained in a previous work. The  $\text{Cm}^{3+}$  ion was found to have the most intense radioluminescence,  $\text{Tb}^{3+}$  and  $\text{Eu}^{3+}$  being slightly weaker. The most probable cause of the disagreement observed between radioluminescence and photoluminescence is the formation of products upon radiolysis which serve to damp the excited states of f-element ions and the variation in effectiveness of radio excitation with atomic number of the element. Figures 2; references 6: 3 Russian, 3 Western.

6508/5915  
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UDC 541.15

RADIATION-CHEMICAL BEHAVIOR OF ACTINIDES IN EXTRACTION SYSTEMS. PART 5.  
 $\text{Pu(IV)} + \text{Zr(IV)}$  IN SYSTEM OF 30% TBP + N-DODECANE UPON  $\gamma$ -RADIOLYSIS

Leningrad RADIOKHIMIYA in Russian Vol 29, No 1, Jan-Feb 87  
(manuscript received 28 May 85) pp 87-92

[Article by M. V. Vladimirova, D. A. Fedoseyev, A. S. Melovanova and I. A. Boykova]

[Abstract] Organic solutions of  $\text{Pu(IV)}$  employed in extraction processing of spent nuclear fuel may contain small quantities of  $\text{Zr(IV)}$ , which may influence the radiation-chemical behavior of the  $\text{Pu(IV)}$  in a system of TBP plus a diluent. This article reports the radiation-chemical behavior of  $\text{Pu(IV)}$  in a system of 30% TBP plus n-dodecane in the presence of  $\text{Zr(IV)}$  as a function of its concentration with absorbed  $\gamma$ -radiation doses of  $2 \cdot 10^4$  to  $4.5 \cdot 10^5$  Gr. The influence of  $\text{Zr(IV)}$  in  $\gamma$ -irradiated organic solutions on the radiation-chemical behavior of  $\text{Pu(IV)}$  is the result primarily of the interaction of  $\text{Zr(IV)}$  with DBPA with the formation of complexes similar to DBP complexes of plutonium. The presence of  $\text{Zr(IV)}$  in organic  $\text{Pu(IV)}$  solutions prevents the formation of  $\text{Pu(IV)} + \text{DBPA}$  complexes. The formation of a plutonium sediment with  $\text{Zr(IV)}$  present begins at a higher  $\gamma$ -radiation dose. The degree of retention of  $\text{Pu(IV)}$  in the organic phase would be expected to decrease with increasing zirconium concentration. Figures 5; references: 5 Russian.

6508/5915  
CSO: 1841/300



CHANGE IN ABSORPTION OF SODIUM-CALCIUM-SILICATE GLASSES OF HIGH PURITY IN THE NEAR IR UNDER INFLUENCE OF  $\gamma$ -RADIATION

Leningrad FIZIKA I KHIMIYA STEKLA in Russian Vol 12, No 6, Nov-Dec 86  
(manuscript received 30 Sep 85) pp 682-690

[Article by L. B. Glebov, V. G. Dokuchayev and G. T. Petrovskiy]

[Abstract] A study was made of the absorption spectra in the 0.7-1.4 eV (0.9-1.8  $\mu$ m) area following  $\gamma$ -radiation of sodium-calcium-silicate high purity glass. The contribution of radiation reduction of iron to this absorption is determined. Studies were performed on a number of glasses containing (mass percent) 75 SiO<sub>2</sub>, 22 Na<sub>2</sub>O and 3 CaO with variable iron content ( $5 \cdot 10^{-5}$ - $3.5 \cdot 10^{-2}$  mass percent). It is found that the additional absorption arising in silicate glasses under the influence of  $\gamma$ -radiation in the 0.7-1.4 eV range is determined by the absorption bands of two hole color centers with maxima at 0.89 and 2.0 eV and radiation-reduced iron. The minimum additional absorption is in the 1.1 eV area (about 1.1  $\mu$ m). The absorption cross sections of each of the color centers and  $[\text{Fe}^{3+}]^-$  and the shape of the absorption bands are determined. A relationship is established between the intensities of additional absorption bands in the visible and UV areas and the additional absorption which arises in the 0.7-1.4 eV region. This allows calculation of the additional absorption in the near IR from the additional absorption in the visible and UV areas. Figures 5; references 13: 11 Russian, 2 Western.

6508/5915

CSO: 1841/304

UDC 541.6+547.1+681.142.2

## UNIVERSAL MACHINE GRAPHICS PROGRAM FOR ORGANIC CHEMISTRY APPLICATIONS

Moscow ZHURNAL VSESOYUZNOGO KHIMICHESKOGO OBSHCHESTVA IM. D. I. MENDELEYEVA  
in Russian Vol 32, No 1, Jan-Feb 87 (manuscript received 27 Mar 86) pp 112-113

[Article by N. S. Zefirov, I. I. Baskin and S. S. Trach, Moscow State  
University imeni M. V. Lomonosov]

[Abstract] Organic structural formulas can be expressed as a matrix of contiguities; these matrices can be combined into complex representations. For storing in computer memory, such structural information can be considered as graphs with atoms at the vertices and chemical bonds as the edges; associated lines and arrows can be expressed as supplementary vertices and edges. Based on this approach, a program entitled "MODEL" and written in Basic has been developed containing approximately 2000 operators divided into functionally independent blocks. This program supports preparation of graphic illustrations and allows the chemist to input data; output it to screen or printer; perform screen editing; input such standard structural elements as rings, chains, and polycyclic systems; separate or combine structural elements; and store the data in magnetic disk files. All symbols and inscriptions are considered as notations of "real" or fictitious vertices, while some 30 types of "real" or fictitious edges represent various types of lines, arrows, etc. Editing can modify these elements or their relation to each other. Output can be in the form of tables combining numerous representations for use with graphic printers. Blocks of the program can also be used to support such associated functions as managing libraries of chemical data and designing synthesis routes. The program is available through the chemical faculty of Moscow State University. Figures 1; references 3: 2 Russian, 1 Western.

12672/5915  
CSO: 1841/274

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